Probability currents as principal characteristics in the statistical mechanics of nonequilibrium steady states

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Abstract. One of the key features of nonequilibrium steady states (NESS) is the presence of nontrivial probability currents. We propose a general classification of NESS in which these currents play a central distinguishing role. As a corollary, we specify the transformations of the dynamic transition rates which leave a given NESS invariant. The formalism is most transparent within a continuous time master equation framework since it allows for a general graph-theoretical representation of the NESS. We discuss the consequences of these transformations for entropy production, present several simple examples, and explore some generalizations, to discrete time and continuous variables.

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1. Introduction.

The characterization and theoretical understanding of non-equilibrium phenomena forms one of the greatest challenges of current statistical physics [1, 2, 3]. In contrast to systems in thermal equilibrium, systems far from equilibrium carry nontrivial fluxes of physical quantities such as particles or energy. These fluxes are induced and maintained by coupling the system to multiple reservoirs, acting as sources and sinks (of particles or energy, say) for the system. Since systems of this type abound in biology, chemistry, and engineering, any progress in this area is likely to have significant impact, well beyond condensed matter physics.

Over the past years, the remarkable richness of non-equilibrium physics has been illustrated beautifully, through the study of simple models. Yet, a satisfactory and comprehensive theoretical framework is still missing, even for the arguably simplest generalizations of equilibrium, namely, non-equilibrium stationary states (NESS). At the source of the difficulties lie several features: First, the evolution of many interesting statistical systems is described by a set of transition rates without the basis of a known, underlying Hamiltonian. Familiar examples span a wide range, e.g., chemical reactions, cell functions, population dynamics, social networks, and financial markets. Second, when (and if) such system reaches a stationary state, it will be a NESS in general.

For such states, there is no *a priori* knowledge of, or a good working hypothesis for, the configurational probability distribution. By contrast, for systems known to reach thermal equilibrium, the fundamental hypothesis is highly successful in providing the stationary distribution, regardless of the details of the dynamical evolution. Finally, seemingly minor modifications of the evolutionary rules (i.e., the system dynamics) often lead to dramatic changes in macroscopic properties, suggesting that *very different* NESS's can be associated with *just slightly different* dynamics.

To appreciate how profoundly NESS differ from equilibrium systems in this regard, let us briefly recall the Gibbs-Boltzmann framework for systems in thermal equilibrium (with a single reservoir). For simplicity, we use the language of the canonical ensemble here [4]. The required inputs are: a set of configurations $\mathcal{C}_1$, $\mathcal{C}_2$, ... of the system (also known as microstates) and an expression for the internal energy $\mathcal{H}(\mathcal{C})$ associated with each configuration $\mathcal{C}$. Then, the statistical weight, $P^{eq}(\mathcal{C})$, for a system in thermal equilibrium with a reservoir is well established, in terms of $\mathcal{H}(\mathcal{C})$ and a simple parameter - temperature T - associated with the reservoir. All macroscopic observables now follow as configurational averages, $\langle A \rangle = \sum_{\mathcal{C}} A(\mathcal{C}) P^{eq}(\mathcal{C})$. In particular, a system coupled to a heat bath at inverse temperature $\beta = 1/k_B T$ is governed by the familiar Boltzmann distribution, $P^{eq}(\mathcal{C}) = Z^{-1} \exp[-\beta \mathcal{H}(\mathcal{C})]$.

Of course, all real systems, whether in equilibrium or not, are fundamentally dynamic in nature, continuously undergoing transitions from one configuration to another. In that context, stationary distributions, including $P^{eq}(\mathcal{C})$, emerge as the long-time limit of a time-dependent distribution, $P(\mathcal{C}; t)$. For its time evolution, we will assume that it obeys a master equation, with a given set of transition rates between the configurations. From a modelling perspective, it is therefore natural to ask: What choices of dynamic transition rates will lead to a desired stationary distribution? and: What modifications of these rates will leave this distribution invariant? For equilibrium systems, the answer is well known and can be traced to the property of *detailed balance*, which is related to *microscopic reversibility*. Specifically, if the rates satisfy detailed balance, the *net* probability current between *any pair* of configurations vanishes in the steady state. As a result, $P^{eq}(\mathcal{C}) \equiv \lim_{t \to \infty} P(\mathcal{C}; t)$ can be expressed in terms of *ratios* of these rates, and the long-time limit remains invariant under any modification of the dynamics which preserves these ratios. Indeed, Monte Carlo simulation studies of equilibrium systems rely heavily on this property. Since the full configurational sum $\sum_{\mathcal{C}}$ is computationally inaccessible, an importance sampling of configuration space is achieved dynamically, by constraining the transition rates such that $P(\mathcal{C}; t)$ eventually approaches the desired equilibrium distribution.

In this article, we begin by addressing two fundamental questions. First, is there a general procedure to find the stationary solution(s) of a master equation even if the transition rates violate detailed balance? Second, can we specify the class of transformations of the rates which leave this stationary distribution invariant? The answer to the first question is not new, expressing the solution in terms of directed trees. Since it does not seem to be widely known, we will provide a brief review here, restricting

ourselves to systems with (i) a finite (but arbitrary) number of configurations, (ii) time-independent transition rates, and (iii) ergodicity. In this framework, we discuss the importance of irreversible loops (associated with the transition rates) in configuration space, the role they play in the non-trivial probability currents, and how equilibrium distributions are recovered in case all loops are reversible. To answer the second question, we proposed [5] a general classification of NESS in terms of the stationary configurational probabilities $P^*(\mathcal{C})$ and the (stationary) probability currents connecting them, $K^*(\mathcal{C}', \mathcal{C})$ - denoted in short by $\{P^*, K^*\}$. A given set $\{P^*, K^*\}$ defines a particular NESS, and allows us to compute all physical currents - mass, energy, etc - for this state. We then discuss the set of transformations of the transition rates which leave $\{P^*, K^*\}$ invariant. In other words, we describe how to generalize the "detailed balance condition" to NESS.

In the reminder of this article, we explore some consequences of our postulate and present several specific examples, to illustrate the very general and formal framework proposed. In a concluding section, we provide a summary and outlook, including some remarks on generalizations to discrete time and continuous configuration space. The Appendices are devoted to technical details.

2. The master equation and its associated steady state

We first establish the mathematical framework for our analysis. Consider a general continuous-time dynamics, with a discrete, finite configuration space. We assume that every configuration can be reached from every other one, so that the system is ergodic. Labelling the configurations in some arbitrary manner as $\mathcal{C}_1$, $\mathcal{C}_2$, .., $\mathcal{C}_N$, we are interested in $P(\mathcal{C}_i; t)$, the probability to find the system in configuration $\mathcal{C}_i$ at time t. Its evolution is governed by a set of transition rates $w(\mathcal{C}_j \rightarrow \mathcal{C}_i)$, for the system to change from configuration $\mathcal{C}_j$ to configuration $\mathcal{C}_i$, per unit time. To simplify notation, let $P_i(t)$ stand for $P(\mathcal{C}_i; t)$ and $w(\mathcal{C}_j \rightarrow \mathcal{C}_i)$ be denoted by w_i^j [6]. All w_i^j are real, non-negative, and assumed to be time-independent. In general, "forward" and "backward" rates differ, i.e., $w_i^j \neq w_j^i$. If one of them vanishes while the other remains nonzero, we will call the corresponding transition uni-directional. In terms of these w's, the master equation simply expresses the rate of change of $P_i(t)$ as the system makes transitions in and out of $\mathcal{C}_i$:

$$\partial_t P_i(t) = \sum_{j \neq i} \left[w_i^j P_j(t) - w_j^i P_i(t) \right] \tag{1}$$

This is often more conveniently written in matrix form

$$\partial_t P_i(t) = \sum_{j=1}^{N} W_i^j P_j(t) \tag{2}$$

where we have introduced the $N \times N$ matrix W via

$$W_i^j = \begin{cases} w_i^j & \\ -\sum_{k \neq j} w_k^j & \end{cases} \quad \text{if} \quad \begin{matrix} i \neq j \\ i = j \end{matrix} \tag{3}$$

We note that W_i^j is a stochastic matrix (in the continuous-time formalism) since it satisfies (i) $W_i^j \geq 0$ for all $i \neq j$, and (ii) $\sum_i W_i^j = 0$ for all j. The second condition ensures that, once normalized, $P_i(t)$ remains so for all subsequent times.

The right hand side of Equation (1) can be expressed in terms of the (net) *probability currents* K_i^j, from configuration $\mathcal{C}_j$ into configuration $\mathcal{C}_i$,

$$K_i^j(t) \equiv w_i^j P_j(t) - w_j^i P_i(t) \tag{4}$$

so that the master equation simply states the conservation of probability: $\partial_t P_i(t) = \sum_{j \neq i} K_i^j(t)$.

Since the dynamics is ergodic, Equation (1) has a unique stationary solution, $P_i^* \equiv \lim_{t \to \infty} P_i(t)$, independent of the initial conditions. This implies that P_i^* is a *right* eigenvector of W with eigenvalue zero. This eigenvalue is non-degenerate so that P_i^* spans the null space of the matrix W_i^j. The associated *stationary currents* are denoted by K^{*j}_i. They satisfy the equality $\sum_{j \neq i} K^{*j}_i = 0$, for all i, i.e., the total probability current into any given configuration vanishes.

In general, P_i^* depends on the chosen rates, w_i^j. When simulating systems in thermal equilibrium, the challenge is to specify a set $\{w_i^j\}$ such that the resulting stationary state equals the desired equilibrium distribution, P_i^{eq}. A well-established procedure is to choose rates which satisfy "detailed balance" (with respect to P_i^{eq}), namely,

$$w_i^j P_j^{eq} - w_j^i P_i^{eq} = 0 \tag{5}$$

for *every pair* $\mathcal{C}_i, \mathcal{C}_j$ of configurations. This relation can be viewed as a constraint on the set of allowable w's. We see immediately that Equation (5) is equivalent to demanding that *all individual currents vanish*, i.e., $(K^{eq})_i^j = 0$ for all $i \neq j$. Conversely, if the dynamics satisfies detailed balance, even if the steady-state distribution is not explicitly known, we can construct P_i^{eq} easily from Equation (5). Furthermore, it is now very easy to determine whether two *different* sets of rates, $\{w_i^j\}$ and $\{\bar{w}_i^j\}$, will generate the same P_j^{eq}: They do if the equalities $w_i^j / w_j^i = \bar{w}_i^j / \bar{w}_j^i$ hold.

Equation (5) seems to imply that P_i^{eq} must be explicitly known in order to test the validity of detailed balance. However, detailed balance is an intrinsic property of the dynamics, expressing a deeper statement on microscopic reversibility and requiring no information about any specific steady-state distribution P_i^{eq}. Known as the Kolmogorov criterion [7, 8, 2, 9], it relies on considering closed loops in configuration space, e.g., $\mathcal{L} \equiv \mathcal{C}_i \to \mathcal{C}_j \to \mathcal{C}_k \to ... \to \mathcal{C}_n \to \mathcal{C}_i$. For each loop, we define the product of the associated rates in the "forward" direction, $\Pi[\mathcal{L}] \equiv w_j^i w_k^j ... w_i^n$, as well as for the "reverse" direction: $\Pi[\mathcal{L}_{rev}] \equiv w_i^j w_j^k ... w_n^i$. In terms of these products, the dynamics is said to satisfy detailed balance if

$$\Pi[\mathcal{L}] = \Pi[\mathcal{L}_{rev}] \tag{6}$$

for *all* loops. This condition implies the *path-independence* of the ratio of the associated products of the rates along *any* path which goes from $\mathcal{C}_i$ to $\mathcal{C}_j$. To be more explicit,

consider a path: $\mathcal{P} \equiv \mathcal{C}_i \to \mathcal{C}_k \ldots \to \mathcal{C}_n \to \mathcal{C}_j$ and its "reverse" $\mathcal{P}_{rev} \equiv \mathcal{C}_j \to \mathcal{C}_n \ldots \to \mathcal{C}_k \to \mathcal{C}_i$. Then, the ratio

$$\Pi_j^i \left[\mathcal{P} \right] \big/ \Pi_i^j \left[\mathcal{P}_{rev} \right] \equiv \frac{w_k^i \ldots w_j^n}{w_n^j \ldots w_i^k} \tag{7}$$

assumes the same value as $\Pi_j^i \left[\mathcal{P}' \right] \big/ \Pi_i^j \left[\mathcal{P}'_{rev} \right]$ where $\mathcal{P}'$ is any other path from $\mathcal{C}_i$ to $\mathcal{C}_j$. Such path independence allows us to define a unique "potential" associated with each $\mathcal{C}_i$:

$$\Phi_{io} \equiv \ln \left(\Pi_i^o / \Pi_o^i \right) \;, \tag{8}$$

where $\mathcal{C}_o$ is some arbitrary reference configuration. As we will demonstrate below, it is straightforward to show that the stationary distribution is then given by

$$P_i^* \propto \exp \left[\Phi_{io} \right] \;. \tag{9}$$

The relationship between this P_i^* and the familiar P_i^{eq} is now clear: The potential Φ is, e.g., just $-\beta \left\{ \mathcal{H} \left[\mathcal{C}_i \right] - \mathcal{H} \left[\mathcal{C}_o \right] \right\}$ for the canonical distribution. Further, for systems obeying Equation (6), this approach allows us to define an effective Hamiltonian $\mathcal{H}_{eff}$ along with an effective (inverse) temperature β_{eff}, in case such concepts are beneficial for the problem at hand.

A key signature of *non*-equilibrium steady states is that the underlying rates do not satisfy microscopic reversibility and Equation (6) is violated. As a result, the ratios Equation (7) will be depend explicitly on the path $\mathcal{P}$. This leads Lebowitz and Spohn to define [10] an action associated with each $\mathcal{P}$ as the log of the ratio (7). In a more specific arena, the dynamic functional [11] is its counterpart in typical statistical field theories.

For a NESS, the right hand side of Equation (5) is generically nonzero, given by the nontrivial stationary probability currents: As a result, the construction of the stationary probability distribution – while still possible – requires a bit more effort. Though established some time ago [12, 13, 14], the graph-theoretical approach, similar to those originally designed for electric networks [15], appears not to be widely known [9]. For the reader's convenience, we briefly review the method here. First, we represent each configuration by a labelled vertex (e.g., i for $\mathcal{C}_i$). Next, we draw all distinct spanning trees (i.e. all distinct graphs containing all vertices and exactly one single undirected edge between each pair so that no loops are formed) t_α, $\alpha = 1, 2, .., M$, with N vertices. The total number of such trees, M, is given by N^{N-2}, according to Cayley's theorem [16]. Next, we select a specific vertex, e.g., i, and draw an arrow, directed towards i, on every edge. The resulting *directed* tree will be denoted by $t_{\alpha(i)}$. Note that, for given i, there is exactly one directed tree for each undirected tree. Next, we associate a factor w_j^k with an edge directed from vertex k to j. Finally, the numerical value $U(t_{\alpha(i)})$ of the directed tree $t_{\alpha(i)}$ is defined to be the product of the $(N-1)$ rates w appearing in that particular tree. If one of the rates vanishes, we simply assign the value $U(t_{\alpha(i)}) = 0$ to the associated tree. We illustrate the procedure in Figure 1 for finding P_1^* in a $N = 4$ case. While we show all 16 directed trees, we just give two of the U's as examples:
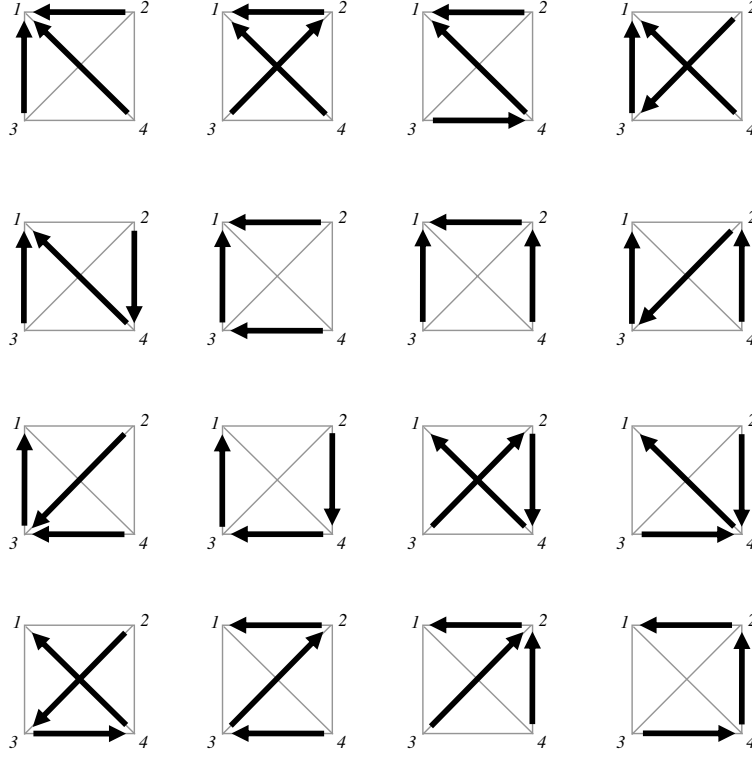
Figure 1. All 16 directed trees contributing to the graphical representation of P_1^*, for a simple model with $N = 4$.

$U(t_{4(1)}) = w_1^4 w_1^3 w_3^2$ (top right diagram in Figure 1) and $U(t_{13(1)}) = w_1^4 w_4^3 w_3^2$ (bottom left diagram in 1). The stationary solution of Equation (1) is then given by

$$P_i^* = \mathcal{Z}^{-1} \sum_\alpha U(t_{\alpha(i)}) \tag{10}$$

with the normalization factor $\mathcal{Z}$ defined as

$$\mathcal{Z} \equiv \sum_{i=1}^N \sum_\alpha U(t_{\alpha(i)}) \tag{11}$$

Now that we have a representation for P_i^*, let us consider the probability currents, defined in Equation (4) above. Specializing to the stationary case, we write the *net* current from $\mathcal{C}_j$ into $\mathcal{C}_i$ in the form:

$$K^{*j}_{\ i} \equiv w_i^j P_j^* - w_j^i P_i^* = \mathcal{Z}^{-1} \sum_\alpha \left[w_i^j U(t_{\alpha(j)}) - w_j^i U(t_{\alpha(i)}) \right] \tag{12}$$

Focusing on the expression within [...], we note that, for a specific α, the trees $t_{\alpha(i)}$ and $t_{\alpha(j)}$ differ only in the directed edges that connect vertices i and j. In Figure 2, we illustrate this statement with a tree that has $k_1, ..., k_\ell$ as the vertices between i to j. In Figure 2a, $t_{\alpha(j)}$ involves a directed tree used for $U(t_{\alpha(j)})$, with directed edges being blue. Similarly, in Figure 2b, we have the same tree being used for $U(t_{\alpha(i)})$, the only difference being the edges *between* i and j which are now reversed. Considering just this segment of the two trees, we may write the associated products of the w's as
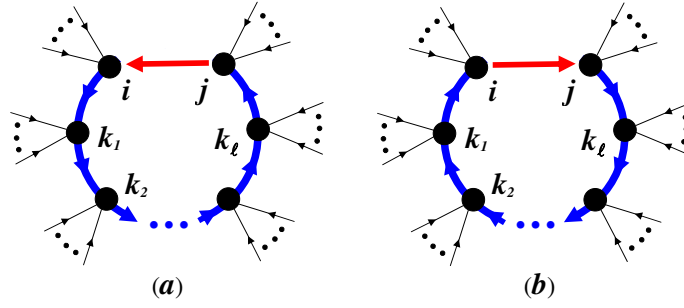
Figure 2. An illustration of the forward and backward loops, appearing in the sum on the right hand side of Equation (12). See text for details.

$\Pi_j^i(t_{\alpha(j)}) = w_{k_1}^i w_{k_2}^{k_1} ... w_j^{k_\ell}$ and $\Pi_i^j(t_{\alpha(i)}) = w_{k_\ell}^j ... w_i^{k_1}$, respectively. Meanwhile, the rest of both trees (the side branches "coming into the circle" in Figure 2) are identical. Thus, denoting the products of the rates associated with these side branches as R, we may write

$$R(t_{\alpha(i)}) = R(t_{\alpha(j)}).$$

Combining the side branches with the path between i and j, we arrive at

$$U(t_{\alpha(j)}) = \Pi_j^i(t_{\alpha(j)})R(t_{\alpha(j)}) \quad \text{and} \quad U(t_{\alpha(i)}) = \Pi_i^j(t_{\alpha(i)})R(t_{\alpha(i)}) \tag{13}$$

Returning to the steady-state current, Equation (12), we see that the additional factor of w in each term can be regarded as adding an extra edge (red), so that each tree is converted into a graph with a *single* loop (the "circles" in Figure 2). It is natural to label these directed loops as $\mathcal{L}_{\alpha(j)}$ and $\mathcal{L}_{\alpha(i)}$ respectively. Of course, both refer to the *same* loop, just traversed in *opposite* directions. Quantitatively, we have, for each t_α

$$w_i^j U(t_{\alpha(j)}) - w_j^i U(t_{\alpha(i)}) = \left\{ w_i^j w_{k_1}^i w_{k_2}^{k_1} ... w_j^{k_\ell} - w_j^i w_{k_\ell}^j ... w_i^{k_1} \right\} R(t_{\alpha(j)}) .$$

Now, the terms in {...} can be associated with $\mathcal{L}_{\alpha(j)}$ and $\mathcal{L}_{\alpha(i)}$, so that a compact expression for the current is

$$K_i^{*j} = \mathcal{Z}^{-1} \sum_\alpha \left[\Pi(\mathcal{L}_{\alpha(j)}) - \Pi(\mathcal{L}_{\alpha(i)}) \right] R(t_{\alpha(i)}) . \tag{14}$$

From here, it is immediately obvious that detailed balance, manifested in reversible loops, Equation (6), will lead to all K_i^{*j} being zero, and nontrivial steady-state currents can only emerge from rates which violate detailed balance. For completeness, we should remark that it is conceivable for accidental cancellations in the sum over trees to occur so that *some* K^*'s may vanish even though irreversible loops are present. However, K^* should be nonzero, generically.

Let us point out briefly that there is an alternate representation of the stationary distribution [9], in terms of the co-factors of W_i^j (which we denote by C_j^i here). Of course, a well known expression of the determinant leads us to $\det W = \sum_j W_i^j C_j^i$ for any i. Moreover, for a stochastic matrix W_i^j, C_j^i is independent of i. Thus, we may write C_j

in place of C_j^i. Finally, since W has a zero eigenvalue, we have $0 = \det W = \sum_j W_i^j C_j$. Thanks to the uniqueness of the stationary solution, this equality implies $C_j \propto P_j^*$.

Before proceeding to the next section, it may be instructive to see how the complex expression for P^*, Equation (10), reduces directly to the familiar form for systems in equilibrium. To start, we choose an arbitrary reference configuration $\mathcal{C}_o$. Of course, we will rely on the path-independent properties of Π_j^o/Π_o^j. Consider the ratio

$$\sum_\alpha U(t_{\alpha(j)}) \left[\sum_\alpha U(t_{\alpha(o)}) \right]^{-1}$$

and exploit the factorization, Equation (13). Then, the numerator of the above reads

$$\sum_\alpha U(t_{\alpha(j)}) = \sum_\alpha \Pi_j^o(t_{\alpha(j)}) R(t_{\alpha(j)}) \ , \tag{15}$$

where $\Pi_j^o(t_{\alpha(j)})$ now stands for the product of the rates associated with the path from $\mathcal{C}_o$ to $\mathcal{C}_j$ in $t_{\alpha(j)}$ and $R(t_{\alpha(j)})$, with the rest of the tree ("side branches"). Of course, we have a similar decomposition for the denominator. Next, we invoke the path independence of the Π's (Equation (8)) and write

$$\Pi_j^o(t_{\alpha(j)}) = \Pi_o^j(t_{\alpha(o)}) e^{\Phi_{jo}} \ .$$

Let us emphasize that Φ_{jo} does *not* depend on the path so that it is also independent of t_α. Consequently, Equation (15) becomes

$$\sum_\alpha U(t_{\alpha(j)}) = e^{\Phi_{jo}} \sum_\alpha \Pi_o^j(t_{\alpha(o)}) R(t_{\alpha(j)}) \ .$$

But, as noted above, the side branches of $t_{\alpha(j)}$ and $t_{\alpha(o)}$ are identical, so that we can replace $R(t_{\alpha(j)})$ by $R(t_{\alpha(o)})$. The sum on the right is easily recognized as $\sum_\alpha U(t_{\alpha(o)})$ and we arrive at

$$\sum_\alpha U(t_{\alpha(j)}) = e^{\Phi_{jo}} \sum_\alpha U(t_{\alpha(o)}) \ .$$

and the desired result for systems in thermal equilibrium:

$$P_i^* = P_o^* \exp\left[\Phi_{io}\right] \ . \tag{16}$$

3. A postulate for the complete characterization of NESS

In much of the literature on NESS, the *microscopic* stationary distribution P^* tends to be the central focus, along with those *macroscopic* properties which can – at least in principle – be derived from it, such as order parameters and correlation functions. In this sense, the investigations follow standard routes for systems in thermal equilibrium. Indeed, many studies emphasize the similarity between the P^* of a NESS and the P^{eq} of an equilibrium system. At the same time, many complementary studies focus on quantities *absent* from equilibrium systems, e.g., particle currents or energy fluxes through the system. Unlike P^*, however, these are *macroscopic* averages, and thus located at the same scale as order parameters and correlation functions. It is natural

to ask whether there is a non-equilibrium quantity, or concept, which would provide a *microscopic* basis for these fluxes. Here, we propose that the microscopic distribution of probability currents, K^*, be brought to stage center, as an indispensable partner for the microscopic probability distribution P^*. Clearly, the particle/energy fluxes can be computed from K^* as averages, on a par with $\langle \bullet \rangle = \Sigma \bullet P^*$. Needless to say, in the arena of *equilibrium* statistical physics, all K^*'s vanish and therefore play the role of an invisible partner.

To showcase the essential nature of K^*, let us consider a completely trivial example, namely, a single particle hopping randomly between neighboring sites on a ring. As long as the rates are spatially uniform, the stationary probability distribution is trivially flat: $P^* \propto 1$, *regardless* of whether the hopping rates are symmetric (i.e., identical for left and right hops) or biased. Yet, detailed balance is satisfied if and only if they are symmetric, and there is an important *physical* difference between the two cases, namely, the presence or absence of a particle current in the stationary state. In more complex cases, other types of currents (e.g., energy) may be the key feature. In general, all these fluxes can be traced to the violation of detailed balance and the associated microscopic probability currents. In other words, without K^*, P^* alone cannot be a complete description of a NESS.

That K^* has been largely ignored in the literature may be traced to the following. In all studies of non-equilibrium systems, we begin with a given set of rates $\{w\}$, motivated by the underlying physics, chemistry, biology, psychology, sociology, etc. The main difficulty is to find P^*. But, once P^* is known, macroscopic average fluxes can be computed easily from w and P^*, so that it is unnecessary to construct K^* explicitly. However, if we wish to ask the *inverse question*, namely: "What rates are needed to *achieve* a particular NESS?", then K^* plays an indispensable role.

Though seemingly trivial, let us state for completeness that K^* alone is also inadequate. Specifically, it is possible to have NESS's with the same K^* but different P^*'s. Electromagnetism provides a good analog. In electrostatics, the central focus is the charge distribution, being the analog of P^*. By definition of electrostatics, there are no currents anywhere. Similarly, we are concerned mainly with the currents in magnetostatics and tend to ignore the charge distribution. However, it is clear that, in general, the charge distribution is not trivial, especially for non-neutral systems.

Staying with electromagnetism for a moment, Kirchhoff's solution for general electric circuits [15] is often quoted as the first graphical solution to the master equation. Yet, there are non-trivial differences. Specifically, the currents (I_{ij} between nodes i and j) are clearly the quantities of interest for Kirchhoff, while there is no trace of the charge distribution (ρ_i at node i) in his solution. In contrast, P^* is the key quantity when solving the master equation. Further, there is no one-to-one mapping from the set of electromotive forces and resistances to the set of rates. Further details regarding the "duality" of our NESS and the Kirchhoff problem may be found in Appendix A.

Motivated by these considerations, we propose that $\{P^*, K^*\}$, the distributions for probability and probability currents, form a *complete and unique* description for

any stationary state. This classification includes equilibrium systems, characterized by $\{P^{eq}, 0\}$, as well as NESS's where K^* is, by definition, non-zero.

The inclusion of K^* in this characterization motivates the definition of the "distance" of a given NESS from equilibrium, namely,

$$|K^*|^2 \equiv \sum_{i,j} (K^{*i}_j)^2 \ . \tag{17}$$

This may provide a quantitative basis for phrases like "near equilibrium" and "far from equilibrium." How useful this concept is remains to be explored. In Section 4.2 below, we will see $(K^{*i}_j)^2$ appearing in a discussion of entropy production.

More importantly, K^* contains all information necessary to determine the average *fluxes* (or currents) associated with physical observables, such as energy or particle number density. A microscopic distribution of probability currents, it serves as the statistical weight in the computation of physical currents. Explicitly, we write

$$\langle \mathcal{J} \rangle \equiv \frac{1}{2} \sum_{i,j} \mathcal{J}\left(\mathcal{C}_i, \mathcal{C}_j\right) K^*\left(\mathcal{C}_i, \mathcal{C}_j\right) \tag{18}$$

where $\mathcal{J}\left(\mathcal{C}_i, \mathcal{C}_j\right)$ is associated with a physical observable. Naturally, we expect physically meaningful $\mathcal{J}$'s to be antisymmetric under $\mathcal{C}_i \Leftrightarrow \mathcal{C}_j$ (e.g., a particle current). Taking advantage of this fact, we can define $\langle \mathcal{J} \rangle$ in a manner that highlights K^* as a probabilistic weight, namely,

$$\langle \mathcal{J} \rangle \equiv \sum_{\{i,j\}} \mathcal{J}\left(\mathcal{C}_i, \mathcal{C}_j\right) K^*\left(\mathcal{C}_i, \mathcal{C}_j\right) \tag{19}$$

where $\{i, j\}$ denotes a sum taken over *only the positive K^*s*. For the readers' convenience, we illustrate these considerations with two examples.

Many NESS models involve particles hopping from a site (labeled by s) to a neighboring site on a lattice, with an excluded volume constraint. A classic example is the totally asymmetric exclusion process (TASEP) [17, 18]. For such models, a configuration is uniquely given by the set of occupation numbers: $\{n_s\}$. Now, one quantity of interest might be the average particle current across a *particular* pair of sites (bond). Specifically, for the current from site a to b, we need

$$\mathcal{J}_{bond}\left(\{n_s\}, \{n'_s\}\right) = n_a \left(1 - n_b\right) \left(1 - n'_a\right) n'_b - n'_a \left(1 - n'_b\right) \left(1 - n_a\right) n_b \tag{20}$$

Clearly, for the net current across, say, some surface in a 3-dimensional system, we only need to sum the $\mathcal{J}$'s associated with bonds which pierce the surface: $\mathcal{J}_{surface}\left(\{n\}, \{n'\}\right) = \Sigma \mathcal{J}_{bond}$. Further, if the entire distribution for this current (denoted by $p\left(\mathcal{J}\right)$) is of interest, then it is given by

$$p\left(\mathcal{J}\right) = \frac{1}{2} \sum_{\{n\},\{n'\}} \delta\left(\mathcal{J} - \mathcal{J}_{surface}\left(\{n\}, \{n'\}\right)\right) K^*\left(\{n\}, \{n'\}\right) \ .$$

Let us reiterate the need for K^* (as opposed to P^*) in finding these physical currents, even though P^* alone may appear to be the only necessary ingredient for computing averages. This paradox can be traced to Equation (4), which allows us access to K^* from
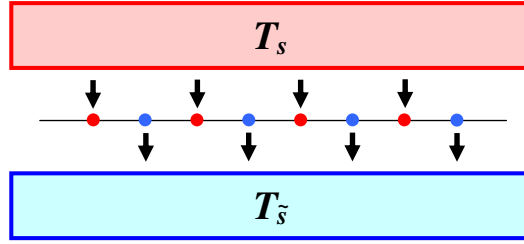
Figure 3. A simple kinetic Ising chain, coupled to two temperature baths. Spins coupled to the higher (lower) temperature are indicated by red (blue) dots. In the steady state, there are constant energy fluxes, as denoted by the black arrows.

P^*, provided the rates $\{w\}$ are known. Typical studies of NESS begin with a given set of rates and unknown $\{P^*, K^*\}$. Thus, the currents are seemingly unimportant, once P^* is found. However, as will be discussed in the next section, there are many w's that can lead to the same $\{P^*, K^*\}$! In this sense, the rates are not *necessary* (though sufficient) for finding average fluxes, and some details of their precise form are "irrelevant."

Another example of a current in a simple NESS is the total energy flux through a kinetic Ising model coupled to two thermal baths at *different* temperatures, as studied in, e.g., [19, 20, 21, 1, 22, 23]. For simplicity, we consider a one-dimensional version here, as shown in Figure 3. Let us denote the set of sites coupled to the two baths by $\{s\}$ and $\{\tilde{s}\}$, respectively, and a particular spin configuration by $\{\sigma_s\}$. We are interested in the energy flowing from the bath at the higher temperature, T_s, to the bath at lower temperature, $T_{\tilde{s}}$. Given the details of the coupling, energy flows into (out of) the system through the $\{s\}$ ($\{\tilde{s}\}$) spins. Using a random sequential dynamics, the energy current operator, in units of the nearest-neighbor coupling strength, can be written as

$$\mathcal{J}_\mathcal{E}\left(\{\sigma_s\}, \{\sigma'_s\}\right) = \sum_s \left(\sigma_{s-1} + \sigma_{s+1}\right)\left(\sigma'_s - \sigma_s\right)\delta_s$$
$$- \sum_{\tilde{s}} \left(\sigma_{\tilde{s}-1} + \sigma_{\tilde{s}+1}\right)\left(\sigma'_{\tilde{s}} - \sigma_{\tilde{s}}\right)\delta_{\tilde{s}} \,,$$

where $\delta_s \equiv \prod_{k \neq s}\left(1 + \sigma_k \sigma'_k\right)/2$ and a similar $\delta_{\tilde{s}}$ insure that only the spin at site s or $\tilde{s}$ is flipped. If the two temperatures are the same and the system is in equilibrium, then $\langle \mathcal{J}_\mathcal{E} \rangle$ is trivially zero due to $K^* \equiv 0$. If we use the rates and P^* instead, a tedious calculation will show that the average of *each term* in $\mathcal{J}_\mathcal{E}$ vanishes.

To summarize, we postulate that $\{P^*, K^*\}$ is a complete characterization of a general NESS. Compared to an equilibrium state, which is specified by $N-1$ quantities (P^*), a NESS requires $O\left(N^2\right)$ quantities. Note that the $N\left(N-1\right)/2$ quantities in K^* are not independent: There are N constraints, namely, $\Sigma_i K^{*i}_{\ j} = 0$. The significance of our characterization is that $\{P^*, K^*\}$ gives access to all macroscopic quantities of interest, including any currents flowing through, or current loops within, the system, without requiring any additional knowledge about the rates. In the following, we explore the consequences of our proposal.

4. Consequences of the postulate

Once a NESS is characterized by $\{P^*, K^*\}$, we can explore the possibility of a generalized "detailed balance condition," which the transition rates must satisfy in order to ensure settling into a given NESS. This freedom of choice has implications for entropy production, as well as for the design of optimized computer simulations.

4.1. Dynamic equivalence classes.

In many investigations of NESS, one of the most striking features is their sensitivity to the details of the transition rates. Major changes of macroscopic properties often emerge from seemingly minor modifications of the rates. It is therefore natural to ask how one might determine whether two sets of rates will lead to the same, or a different, NESS. This issue can be addressed within the framework proposed here. In particular, since all properties of a NESS are supposedly given by $\{P^*, K^*\}$, all *time-independent* (static) quantities of physical interest can be computed, *without* further recourse to the dynamics [24]. The analog in equilibrium systems is that all (static) quantities can be obtained from P^* without detailed knowledge of the rates.

An alternate phrasing of the above question is: Given a set of w's and its associated NESS, what are the transformations on the rates which leave this $\{P^*, K^*\}$ invariant? For the equilibrium case, $\{P^{eq}, 0\}$, the answer is provided by the detailed balance condition, Equation (5): Any set of w's will lead to the desired P^{eq}, provided $w_i^j / w_j^i = P_i^{eq} / P_j^{eq}$. Alternatively, this relation can be interpreted as a constraint to be placed on the rates if the goal is to reach a specific P^{eq}. In our framework, this constraint can now be easily generalized: To arrive at a *given* $\{P^*, K^*\}$ final state, the w's must satisfy

$$w_i^j P_j^* - w_j^i P_i^* = K_i^{*j} \ . \tag{21}$$

for all pairs $i \neq j$. As a simple extension of the equilibrium case (Equation 5), this equation constrains, say, the "backward" rate w_j^i once an (arbitrary or suitable) "forward" rate w_i^j is selected. In this sense, there is just as much freedom in choosing rates to arrive at a given NESS as for systems to reach thermal equilibrium. In the following, we will explore alternative expressions for this simple constraint, to provide further insight.

Motivated by the antisymmetric nature of the currents K_i^{*j}, we define

$$\bar{W}_i^j \equiv W_i^j P_j^* \tag{22}$$

and decompose it into its symmetric and antisymmetric parts:

$$\bar{W}_i^j = S_i^j + A_i^j \ , \tag{23}$$

where $S_i^j \equiv (\bar{W}_i^j + \bar{W}_j^i)/2$, and $A_i^j \equiv (\bar{W}_i^j - \bar{W}_j^i)/2$. Then, Equation (21) is a very simple constraint, namely,

$$A_i^j = \frac{1}{2} K_i^{*j} \ . \tag{24}$$

As a result, for a given $\{P^*, K^*\}$, A is completely determined. In contrast, S is essentially free, except for two restrictions. First, the physical rates must be non-negative ($w \geq 0$), leading to $S_i^j \geq |A_i^j|$, for all $i \neq j$. Further, probability conservation imposes $\sum_i W_i^j = 0$, for all j, so that $\sum_i \bar{W}_i^j = 0$ also. Now, $\sum_i A_i^j$ also vanishes, since $\sum_i (\bar{W}_i^j - \bar{W}_j^i) = -\sum_i W_j^i P_i^*$, which is zero by virtue of $\partial_t P_j^* = 0$. Therefore, $\sum_i \bar{W}_i^j = 0$ reduces to $\sum_i S_i^j = 0$ and we arrive at the restrictions for S:

$$S_i^j \geq \frac{1}{2}\left|K^{*j}_{\ i}\right| \quad \forall i \neq j, \qquad S_j^j = -\sum_{i \neq j} S_i^j . \tag{25}$$

Within these constraints, we may choose *arbitrary* S's, construct transition rates via

$$W_i^j = \left[S_i^j + \frac{1}{2}K^{*j}_{\ i}\right](P_j^*)^{-1} \quad , \tag{26}$$

and be certain that the final NESS remains unaffected. In this respect, we may regard all such S's - specified by $N(N-1)/2$ parameters - as generating an "equivalence class" of dynamic rates associated with the *same* NESS.

There is another, perhaps simpler, way to express this freedom of choice. Suppose we found P^* from a given set of rates w_i^j (and so, K^* is also determined). To construct another set of equivalent rates, it is sufficient to *add* to the w's any set of changes Δ that satisfy

$$\Delta_i^j P_j^* = \Delta_j^i P_i^* . \tag{27}$$

Note that Δ may be *negative*, provided the new rates $w_i^j + \Delta_i^j$ are non-negative. Of course, this amounts to the same statement as Equation (25). Equation (27) is reminiscent of the "ordinary detailed balance" condition. The distinguishing feature here is that the *differences* between two sets of rates, as opposed to the rates themselves, must satisfy "detailed balance with respect to P^*."

Another interesting corollary allows us to determine (some aspects of) P^* from *two* different sets of rates w, w' provided we know that both lead to the same NESS. The key is to compute the differences: $\Delta = w - w'$. For all nonvanishing pairs $\{\Delta_i^j, \Delta_j^i\}$, the ratio can be used to construct P^*. In this sense, the Δ's can be thought of as 'rates that lead to an *equilibrium* state', satisfying microscopic reversibility, Equation (6). Two features distinguish this case from a true equilibrium system: (a) Some Δ's can be negative and (b) there is a unique P^* even if the Δ's are not ergodic (i.e., not all configurations connected by Δ's).

Lastly, let us present an alternate approach. For equilibrium steady states, instead of considering $\bar{W}$, it is more convenient to define another matrix, namely,

$$\tilde{W}_i^j \equiv W_i^j \left(P_j^*/P_i^*\right)^{1/2} \tag{28}$$

Due to detailed balance, $\tilde{W}$ is symmetric, and the master equation is transformed into a standard eigenvalue problem. Apart from a single zero eigenvalue (associated with P^{eq}), all other eigenvalues are negative. Clearly, we can also consider the properties of $\tilde{W}$ in the non-equilibrium case. Similar to $\bar{W}$, $\tilde{W}$ can be decomposed into a symmetric ($\tilde{S}$)

and a *nonzero* asymmetric part, $\tilde{A} = \tilde{K}^*/2$. Here, $\tilde{K}^*$ is related to the original currents K^* via

$$\tilde{K}^{*j}_{\ i} \equiv K^{*j}_{\ i} \left(P^*_j P^*_i \right)^{-1/2} \qquad . \tag{29}$$

For the NESS, we can still conclude, thanks to the Perron-Frobenius theorem, that there is only a single zero eigenvalue, and that all other eigenvalues have strictly negative real parts. However, the eigenvalues need no longer be real and may appear in complex conjugate pairs. These correspond to oscillatory relaxation, as in underdamped oscillators.

Similar to our approach above, for a given NESS, $\tilde{A}$ is completely determined while $\tilde{S}$ is essentially arbitrary (apart from the minor restrictions imposed by positivity and normalizability). The two approaches have complementary advantages: $\bar{W}$ provides immediate information on the probability currents. $\tilde{W}$ has the same spectrum as the original W, and therefore reflects the dynamics more clearly.

We conclude this section by emphasizing that W matrices belonging to an equivalence class have, in general, a different set of nonzero eigenvalues. Needless to say, the physical interpretation is that *different* rates generally lead to *different* relaxation rates into the *same* NESS. Indeed, our hope is that future Monte Carlo simulations of the NESS will exploit this freedom to devise more efficient algorithms, in the same spirit as, say, the cluster algorithms [25], designed specifically to circumvent critical slowing-down in equilibrium systems near critical points.

4.2. Entropy production

One of the key signatures of non-equilibrium steady states, recognized many decades ago [26, 13, 27], is entropy production. Using the expression for average fluxes above (Equation 18), one possible definition [13] for the total entropy production is:

$$\dot{\mathbf{S}}_{tot}(t) \equiv \frac{1}{2} \sum_{i,j} K^j_i(t) \ln \frac{W^j_i P_j(t)}{W^i_j P_i(t)} \ . \tag{30}$$

If the master equation is interpreted in the language of chemical reactions, $\ln \left(W^j_i P_j / W^i_j P_i \right)$ would be an affinity, or generalized "thermodynamic force" [13]. Inserting Equation (4) for $K^j_i(t)$, it is immediately apparent that $\dot{\mathbf{S}}_{tot}(t) \geq 0$. Further, $\dot{\mathbf{S}}_{tot}$ can be written as the sum of two terms, i.e., the entropy production of the "system" and of the "medium",

$$\dot{\mathbf{S}}_{sys}(t) \equiv \frac{1}{2} \sum_{i,j} K^j_i(t) \ln \frac{P_j(t)}{P_i(t)} \ , \ \ \dot{\mathbf{S}}_{med}(t) \equiv \frac{1}{2} \sum_{i,j} K^j_i(t) \ln \frac{W^j_i}{W^i_j}. \tag{31}$$

The former is readily recognized as the time derivative of $\mathbf{S}_{sys} \equiv -\sum_i P_i(t) \ln P_i(t)$, which motivates the term "entropy production of the system". The latter is attributed to the coupling of the system to the *external environment* in a manner that prevents it from reaching equilibrium [13]. Unlike $\dot{\mathbf{S}}_{tot}$, neither $\dot{\mathbf{S}}_{sys}$ nor $\dot{\mathbf{S}}_{med}$ are necessarily positive.

Since we are primarily interested in steady states, we take the infinite time limit. For equilibrium systems, all K^{*j}_i are identically zero so that both $\dot{\mathbf{S}}_{sys}$ and $\dot{\mathbf{S}}_{med}$ vanish. For a NESS, however, only $\dot{\mathbf{S}}^*_{sys}$ vanishes. In general, $K^* \neq 0$ leads to $\dot{\mathbf{S}}^*_{med} = \dot{\mathbf{S}}^*_{tot} > 0$. The interpretation of these results is clear: In the steady state, the entropy associated with the system no longer changes. However, being coupled in an irreversible way to the environment, a NESS continues to increase the entropy of its surrounding medium. In other words, $\dot{\mathbf{S}}^*_{med}$ carries information about the precise nature of these couplings, encoded in the transition rates. So, even if we insist on having the same NESS (i.e., a given $\{P^*, K^*\}$), $\dot{\mathbf{S}}^*_{med}$ will not be unique. In the following, we explore the connection between $\dot{\mathbf{S}}^*_{med}$ and the transition rates in more detail.

In the steady state, $\dot{\mathbf{S}}^*_{tot} = \dot{\mathbf{S}}^*_{med}$. Recalling the decomposition of WP^* into a symmetric and an antisymmetric component, Equation (23), it is more convenient to work with $\dot{\mathbf{S}}^*_{tot}$ whence

$$\dot{\mathbf{S}}^*_{tot} = \frac{1}{2} \sum_{i,j} K^{*j}_i \ln \frac{W^j_i P^*_j}{W^i_j P^*_i} = \frac{1}{2} \sum_{i,j} K^{*j}_i \ln \frac{S^j_i + A^j_i}{S^j_i - A^j_i} \ . \tag{32}$$

While the antisymmetric component is fixed by the currents, $A = K^*/2$, the symmetric part S can be chosen at will, as long as it satisfies Equation (25). In particular, while $\dot{\mathbf{S}}^*_{tot} > 0$ has to remain valid for any choice of S, it is possible to make the entropy production arbitrarily small or infinitely large. In other words, exploiting the freedom in the choice of the transition rates, we can select an *arbitrary* value of $\dot{\mathbf{S}}^*_{tot}$, without affecting the underlying NESS $\{P^*, K^*\}$. Let us provide a few details.

To achieve an arbitrarily small $\dot{\mathbf{S}}^*_{tot}$, we only need $S \gg A$, for every non-vanishing element. Expanding Equation (32) to lowest order in $A^j_i / S^j_i = K^{*j}_i / (2S^j_i)$, we arrive at

$$\dot{\mathbf{S}}_{tot} = \sum_{i,j} \frac{\left(K^{*j}_i\right)^2}{2S^j_i} \left[1 + O\left(\frac{K^*}{S}\right)^2 \right] \tag{33}$$

Of course, even though $\dot{\mathbf{S}}^*_{tot}$ can be made arbitrarily small, it still remains strictly positive, retaining the NESS signature thanks to $\left(K^{*j}_i\right)^2$ being strictly positive. Since $\dot{\mathbf{S}}_{med} = \dot{\mathbf{S}}_{tot} = 0$ characterizes an equilibrium system, minimizing $\dot{\mathbf{S}}^*_{tot}$ (for a given NESS) corresponds to selecting rates which are as "equilibrium-like" as possible.

At the opposite extreme, we can construct rates with "infinite" $\dot{\mathbf{S}}^*_{med}$ by reducing at least one off-diagonal S^j_i to $\left|A^j_i\right|$, so that either $S^j_i + A^j_i$ or $S^j_i - A^j_i$ vanishes (but never both). Translating this back into a new matrix of transition rates, via Equation (26), the corresponding transition is now uni-directional, in that one of the two directed edges between the associated pair of configurations is *missing*. Of course, it is possible to make all rates uni-directional, which may be naturally referred to as "maximally asymmetric." Such systems appear frequently in the literature, a particularly familiar example being the totally asymmetric exclusion processes (TASEP) [17, 18]. One clear advantage of having maximally asymmetric rates for all edges is that the number of nontrivial trees contributing to P^* is kept at the absolute minimum. Needless to say, the expression for
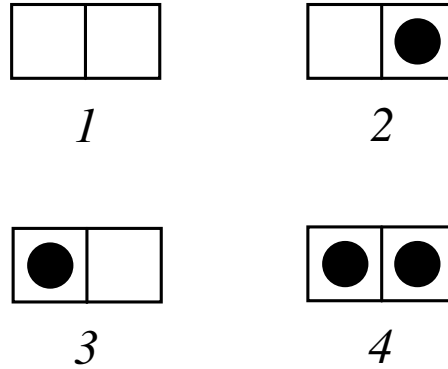
Figure 4. All configurations of a TASEP on a one-dimensional lattice with just two sites. Particles are denoted by black circles.

K^* also simplifies, to just one term in Equation (12), and all irreversible loops are also uni-directional.

5. Examples

The formalism we presented is quite general. It is instructive to provide a series of simple examples, to illustrate how it applies in various circumstances. We will start with a *minute* system, a special case of the $N = 4$ example of 2. It is closely associated with the zero range process (ZRP) and its generalizations which we consider in the second subsection. The third subsection is devoted to a kinetic Ising model coupled to two thermal baths at different temperatures. Finally, we close with the general class of NESS with Gaussian distributions.

5.1. TASEP with two sites

The totally asymmetric exclusion process (TASEP) on a one-dimensional chain with open boundaries [17, 18] enjoys considerable attention as a non-trivial system with a known NESS distribution. The dynamical rules are as follows: Particles may enter (leave) a lattice with L sites at the left (right) end with rate α (β), provided the first (last) site is empty (occupied). Within the system, particles may hop to the right, with rate γ, provided the target site is empty. Though most of the interesting properties appear in the thermodynamic limit, our goal here is to illustrate the considerations of the previous sections. For that purpose, it is more helpful to study a small system. To ensure that nontrivial loops can exist in configuration space, the smallest 'interesting' TASEP is the one with two sites ($L = 2$) and 4 configurations. Let us label these as follows: 1 (4) for both sites being empty (full) and 2 (3) for only the right (left) site being occupied (Figure 4). In Figure 5(a), we show all the allowed transitions (arrows). The rates are α, β, and γ for the vertical (blue), horizontal (green), and diagonal (black)
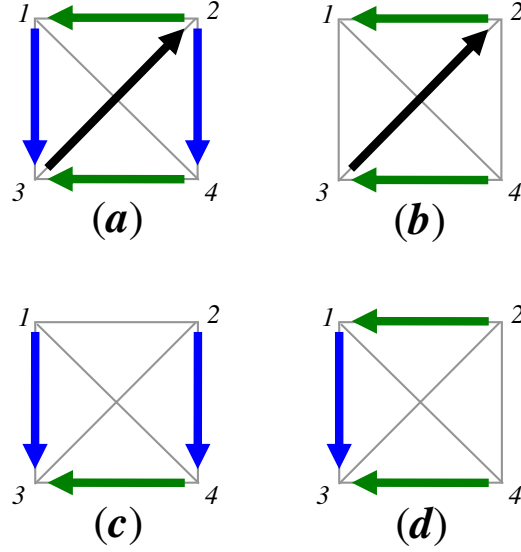
Figure 5. For a TASEP with two sites, all non-vanishing w_j^i are indicated by arrows in (a). (b) The only directed tree contributing to P_1^*. (c,d) The two directed trees contributing to P_3^*.

arrows. The associated matrix W rates can be written easily:

$$W = \begin{pmatrix} -\alpha & \beta & 0 & 0 \\ 0 & -(\alpha+\beta) & \gamma & 0 \\ \alpha & 0 & -\gamma & \beta \\ 0 & \alpha & 0 & -\beta \end{pmatrix}. \tag{34}$$

Note that it is "maximally asymmetric", in concordance with every transition being unidirectional. As a result, most of the 16 possible trees (cf. Figure 1) do not contribute to the graph-theoretical representation of the stationary probabilities P_i^*. For example, only a single tree remains in the representation of P_1^* (shown in Figure 5(b)), and only two trees (Figures 5(c) and 5(d)) remain for P_3^* (see Appendix B for details). The nonvanishing trees are easily found: $P_{1,2,3,4}^* \propto \beta\gamma\beta, \alpha\beta\gamma, \alpha\alpha\beta + \beta\beta\alpha, \alpha\gamma\alpha$. For clarity, let us write the normalized P^* in dimensionless form:

$$P^* = Z^{-1} \begin{pmatrix} \beta/\alpha \\ 1 \\ \alpha/\gamma + \beta/\gamma \\ \alpha/\beta \end{pmatrix} \tag{35}$$

where $Z = 1 + \alpha/\beta + \beta/\alpha + \alpha/\gamma + \beta/\gamma$ differs from $\mathcal{Z}$ in Equation (10) by a factor of $\alpha\beta\gamma$. The stationary probability currents can be easily computed from here. There are only two independent ones, e.g., $K_4^{*2} = \alpha/Z$ and $K_1^{*2} = \beta/Z$. For these simple currents, there is only one associated graph, each with an irreversible loop, illustrating Equation (14). Again, the details are in Appendix B.

Turning to the dynamic equivalence classes associated with this process, the simplest is to add an arbitrary Δ that satisfies Equation (27), with 6 free parameters

(denoted by $\epsilon_{1,...,6}$ here):

$$\Delta = \begin{pmatrix} -\left(\epsilon_1 + \epsilon_2 + \epsilon_3\right)\frac{\alpha}{\beta} & \epsilon_1 & \epsilon_2\frac{\gamma}{\alpha+\beta} & \epsilon_3\frac{\beta}{\alpha} \\ \epsilon_1\frac{\alpha}{\beta} & -\left(\epsilon_1 + \epsilon_4 + \epsilon_5\right) & \epsilon_4\frac{\gamma}{\alpha+\beta} & \epsilon_5\frac{\beta}{\alpha} \\ \epsilon_2\frac{\alpha}{\beta} & \epsilon_4 & -\left(\epsilon_2 + \epsilon_4 + \epsilon_6\right)\frac{\gamma}{\alpha+\beta} & \epsilon_6\frac{\beta}{\alpha} \\ \epsilon_3\frac{\alpha}{\beta} & \epsilon_5 & \epsilon_6\frac{\gamma}{\alpha+\beta} & -\left(\epsilon_3 + \epsilon_5 + \epsilon_6\right)\frac{\beta}{\alpha} \end{pmatrix}$$

Being the most general Δ, the new transition matrix $W+\Delta$ does not provide transparent insight. Nevertheless, we can draw some interesting conclusions. For example, while the spectrum of W is complex for some α, β, and γ, the spectrum of $W + \Delta$ will be real for sufficiently large ϵ's. Details for the case with only $\epsilon_4 \neq 0$ are found in Appendix B. While this modification corresponds to the rather innocuous addition of backwards hops for the particle, more drastic changes can be made, such as ϵ_3 which allows particle pair creation/annihilation transitions! We reemphasize that, in all cases, none of these modifications will affect the NESS distribution of probabilities or their currents.

Finally, we illustrate the effect of Δ on entropy production. Since the original W does not allow "backwards" transitions, the production rate is infinite. The addition of Δ changes this result to

$$\dot{\mathbf{S}}^*_{tot} = Z^{-1}\left\{\beta\ln\left(1 + \beta/\epsilon_1\right)\left(1 + \beta/\epsilon_2\right) + \alpha\ln\left(1 + \alpha/\epsilon_5\right)\left(1 + \alpha/\epsilon_6\right)\right.$$
$$\left. + \left(\alpha + \beta\right)\ln\left(1 + \left(\alpha + \beta\right)/\epsilon_4\right)\right\} . \tag{36}$$

Interestingly, this quantity is independent of ϵ_3, a result that follows from the lack of transitions between configurations 1 and 4 in the original dynamics.

5.2. Models of mass transport

Motivated by a wide range of physical problems, simple models of mass transport have been introduced. As extensions of TASEP, these models are defined by more general rates for moving masses from site to site. Recently, the exact steady-state distribution for a large class of such models was found, so that they serve as good illustrations of the framework presented above. Here, we will consider the most elementary model, the zero range process (ZRP) [28]: discrete (but otherwise arbitrary) masses transported around a ring of discrete sites. Specifically, let each site s $(s = 1, ..., L)$ of a periodic one-dimensional lattice be occupied by an integer valued mass m_s so that a configuration, $\mathcal{C}_i$ or just i, is specified by the set $\{m_s\}$. Thus, $w_i^j P_j^*$ in Equation (12) would assume the form $P^*\left(\{m_s\}\right)w\left(\{m_s\} \rightarrow \{m'_s\}\right)$. In the random sequential updating version, a transport event takes place during an infinitesimal time interval dt, at some site k: A portion, μ, is chipped off from m_k and added to m_{k+1}, according to a given conditional rate $q\left(\mu|m_k\right)$. In other words, the transitions $w\left(\{m_s\} \rightarrow \{m'_s\}\right)$ connect only configurations with all m's being identical *except* for a single pair. To be explicit, we have,

$$m_s = m'_s \quad \text{for} \quad s \neq k, k+1 \tag{37}$$

while

$$m_k - m'_k = \mu; \quad m_{k+1} - m'_{k+1} = -\mu \tag{38}$$

occurs with rate $q(\mu|m_k)$. This particular "element" in $P^*(\{m_s\}) \, w(\{m_s\} \to \{m_s'\})$ is just

$$q(m_k - m_k'|m_k) P^*(\{m_s\}) \delta(m_k + m_{k+1}, m_k' + m_{k+1}') \prod_{s \neq k, k+1} \delta(m_s, m_s'),$$

where $\delta(\bullet, \bullet)$ is the Kronecker delta. Clearly, the total mass $M \equiv \sum_s m_s$ is conserved and, with finite L as well, the configuration space is both discrete and finite.

In general, finding P^* from a given q can be quite difficult. Fortunately, it can be found for a wide class of such models [29]: If (and only if) $q(\mu|m)$ can be cast in the form

$$q(\mu|m) = g(\mu) f(m - \mu) / f(m), \tag{39}$$

where g, f are two arbitrary positive functions, then P^* is factorizable. Explicitly, $P^*(\{m_s\}) = Z^{-1} \prod_s f(m_s)$, where $Z \equiv \sum_{\{m_s\}} \delta(M, \sum_s m_s) \prod_s f(m_s)$ is a normalization factor. In configuration space (hypercubic L-dimensional lattice $\{m_s\}$), the steady-state current

$$K^*(\{m_s\} \to \{m_s'\}) = P^*(\{m_s\}) \, w(\{m_s\} \to \{m_s'\}) - P^*(\{m_s'\}) \, w(\{m_s'\} \to \{m_s\}) \tag{40}$$

can exist only on planes spanned by m_k and m_{k+1}, i.e., those specified by Equations (37) and (38). The expressions reduce considerably, since the f's from q and P^* cancel.

If $m_k > m_k'$, then the current is easily understood as the result of moving $\mu > 0$:

$$K^*\left(m_k, m_{k+1} \to m_k', m_{k+1}'\right) = Z^{-1} g(\mu) f(m_k - \mu) \prod_{s \neq k} f(m_s)$$

$$= Z^{-1} g(m_k - m_k') f(m_k') \prod_{s \neq k} f(m_s)$$

Alternatively, we can keep P^* implicit and write

$$K^*\left(m_k, m_{k+1} \to m_k', m_{k+1}'\right) = g(m_k - m_k') \frac{f(m_k')}{f(m_k)} P^*(\{m_s\}) .$$

In either case, a simple mnemonic for K^* is: "Replace $f(m_k)$ by $g(m_k - m_k') f(m_k')$ in P^*." For completeness, we should point out that, for $m_k < m_k'$, there is no transition across the $(k, k+1)$ bond, of course. However, the *net current* is still non-trivial, due to the *difference* of terms in Equation (40). Thus, we write

$$K^*\left(m_k, m_{k+1} \to m_k', m_{k+1}'\right) = -Z^{-1} g(m_k' - m_k) f(m_k) \prod_{s \neq k} f(m_s')$$

$$= -g(m_k' - m_k) \frac{f(m_k)}{f(m_k')} P^*(\{m_s'\}) .$$

A more general version of this system, highlighting other subtleties of mass transport models, can be found in Appendix C.

Before ending this subsection, let us illustrate how Equation (27) can be exploited here, to define other transition rates which will lead to the same $\{P^*, K^*\}$. Since P^* is explicitly known, we can easily add further mass transports events without altering the final NESS. For example, in addition to chipping μ from m_k and moving it to m_{k+1}

as above, we may chip off amount of mass, $\tilde{\mu}$, from some other site, ℓ, and move it to another site, ℓ', with an arbitrary rate $\tilde{w}$, *provided* that we also make the reverse move with rate $\tilde{w} f\left(m_\ell - \tilde{\mu}\right) f\left(m_{\ell'} + \tilde{\mu}\right) / f\left(m_\ell\right) f\left(m_{\ell'}\right)$, according to Equation (27). Of course, $\tilde{\mu}$ cannot be completely arbitrary, since it must lie within $[0, m_\ell]$. Further, *many* masses can be chipped off at various sites and moved *simultaneously* (i.e., allowing moves away from planes in the L-dimensional space), so that almost arbitrary configuration changes can take place. The NESS, as we characterize it, will remain invariant provided the reverse moves occur with a rate obeying Equation (27). It is clear that such "long-ranged" moves will be much more efficient in Monte Carlo simulations of the true P^*. This is especially critical for systems that display a condensate, since, on the one hand, P^* is translationally invariant (or totally symmetric under permutations of s), while, on the other hand, typical configurations are associated with a condensate located at a *particular* site. With the original rates, the tunneling times for the condensate to "move" from one site to another, required to restore the invariance of the true P^*, are prohibitively long [30]. In contrast, with arbitrarily long range jumps in configuration space, it is possible to design transition rates that readily sample the symmetric P^*. In this sense, such transitions are comparable to the cluster algorithms which proved so useful in simulation studies of equilibrium systems [25].

5.3. Ising models coupled to two thermal baths

Since its inception 80 years ago, the static Ising model has attracted the spotlight of equilibrium statistical physics. To simulate *dynamic* behavior when the system is coupled to a thermal reservoir, many researchers proposed an assortment of transition rates that, not surprisingly, obey detailed balance 'with respect to' the famous equilibrium distribution. The two most important classes are physically motivated: Glauber dynamics [31] involving flips of individual spins and Kawasaki spin-exchange [32] which conserves the total magnetization (or particle number, in the lattice gas formulation). Given that this model is so well studied in equilibrium, it offers itself naturally to investigations of *non*-equilibrium steady states. Since the 80's, a large variety of rates that *violate* detailed balance have been introduced, leading to an extremely rich array of NESS-Ising models. The uniformly driven lattice gas [33, 1], based on Kawasaki dynamics, is a prime example. Another class of such NESS is the two-temperature Ising model. Based on Glauber spin-flip dynamics, it is coupled to thermal baths at *two* different temperatures [19, 20, 1]. Needless to say, multiple baths can also be considered, but we focus on just two, for simplicity. Even with this restriction, the possible implementations of such couplings are seemingly endless [21, 1]. For our purposes here, we consider a one-dimensional chain with spins coupled alternately to the two baths. The advantage of this model is that, in the steady state, *all* correlations are known [23] and energy fluxes through the system have been computed [21]. Indeed, the full time-dependence is also accessible [34]!

As before, we denote the sites of a periodic one-dimensional lattice by s ($s =$

$1, ..., L$). Each site carries an Ising spin σ_s, so that a configuration, $\mathcal{C}_i$ or just i, is specified by the set $\{\sigma_s\}$ (or just $\{\sigma\}$). Of course, the energy of a configuration is given by the usual form: $-J\sum_s \sigma_s\sigma_{s+1}$. Choosing, for convenience, an even L, we couple the spins at the even/odd sites to two different thermal reservoirs, with temperatures

$$T_e \equiv T_{even\ s} \neq T_{odd\ s} \equiv T_o. \tag{41}$$

Using specifically heat bath dynamics, the master equation for this system can be written as

$$\partial_t P\left(\{\sigma\}, t\right) = \sum_{\{\sigma'\}} \left[w\left(\{\sigma'\} \to \{\sigma\}\right) P\left(\{\sigma'\}, t\right) - w\left(\{\sigma\} \to \{\sigma'\}\right) P\left(\{\sigma\}, t\right)\right] \tag{42}$$

where

$$w\left(\{\sigma'\} \to \{\sigma\}\right) = w_0 \sum_s \left\{\frac{1}{2}\left[1 + \gamma_s\sigma_s\frac{\sigma'_{s-1} + \sigma'_{s+1}}{2}\right]\prod_{j\neq s}\delta\left(\sigma_j, \sigma'_j\right)\right\},$$

and

$$\gamma_s \equiv \tanh\frac{2J}{k_B T_s},$$

and w_0 just sets a scale. Note that this dynamics is quite special, since the transition rates w are independent of the state of the spin to be flipped. Furthermore, with random sequential updates, only a single spin is affected at a time. Thus, the probability currents exist only along the "edges" of an 2^L-dimensional cube (the corners of which represent the full configuration space). To proceed, it is useful to define a spin-flip operator $\mathcal{F}_s$, acting on a spin configuration $\{\sigma\}$:

$$\mathcal{F}_s\{\sigma\} \equiv \{...\sigma_{s-1}, -\sigma_s, \sigma_{s+1}, ...\}$$

which just flips the spin at site s. Now, we can write the net stationary currents, e.g.,

$$K^*\left(\{\sigma\} \to \mathcal{F}_s\{\sigma\}\right) = \frac{w_0}{2}\left[1 - \gamma_s\sigma_s\frac{\sigma_{s-1} + \sigma_{s+1}}{2}\right]P^*\left(\{\sigma\}\right)$$

$$- \frac{w_0}{2}\left[1 + \gamma_s\sigma_s\frac{\sigma_{s-1} + \sigma_{s+1}}{2}\right]P^*\left(\mathcal{F}_s\{\sigma\}\right). \tag{43}$$

In the limit $T_{even\ s} \to T_{odd\ s}$, all the γ's are the same and $P^*\left(\{\sigma\}\right) \propto \exp\left[(J/k_B T)\sum_s \sigma_s\sigma_{s+1}\right]$, so that $K^* \equiv 0$. For the *non*-equilibrium case, a simple and compact form for $P^*\left(\{\sigma\}\right)$ is yet to be discovered. In particular, from the known correlations, we can deduce that the "effective Hamiltonian" would involve long range interactions [22]. Probably the most convenient representation, due to Hilhorst [35], is

$$P^*\left(\{\sigma\}\right) = \frac{1}{1 + \lambda^L}\sum_{\{\tau\}}\left[\prod_s\frac{1 + \lambda\tau_s\tau_{s+1}}{2}\right]\left[\prod_{even\ s}\frac{1 + h_e\tau_s\sigma_s}{2}\right]\left[\prod_{odd\ s}\frac{1 + h_o\tau_s\sigma_s}{2}\right]. \tag{44}$$

where

$$\lambda \equiv \tanh\left[\frac{1}{2}\tanh^{-1}\sqrt{\gamma_e\gamma_o}\right] \quad \text{and} \quad h_{e,o} \equiv \sqrt{(\gamma_e + \gamma_o)/2\gamma_{o,e}}.$$

Note that this representation requires performing a configuration-like sum over an auxiliary set of spins $\{\tau\}$, so that it resembles the partition function for a one-dimensional Ising chain in an inhomogeneous magnetic field. Thus, it is quite involved to find the probability currents K^*. Not surprisingly, they are not zero in general. Deferring details to elsewhere, let us provide some illustrations here.

If the neighboring spins are opposite ($\sigma_{s-1} \neq \sigma_{s+1}$), the transition rates, w, for flipping σ_s are the same in both directions. For an equilibrium system, such a local environment implies $P^*(\{\sigma\}) = P^*(\mathcal{F}_s\{\sigma\})$, so that the steady-state current is trivially zero. By contrast, we can show [36] that

$$P^*(\{\sigma\}) \neq P^*(\mathcal{F}_s\{\sigma\})$$

for, e.g., the configuration $\{\sigma\}$: $\sigma_{s-1} = -1$ with *all* other spins positive, when $T_{even\ s} \neq T_{odd\ s}$. Thus, the net current $K^*(\{\sigma\} \to \mathcal{F}_s\{\sigma\})$ is non-zero. Of course, it is proportional to the difference of the two temperatures and vanishes in the equilibrium limit. Its explicit form is rather complex without being especially illuminating, and will not be displayed here [36]. Instead, let us present the *sum* of these currents, over all spins *not involved*, i.e., $\{\bar{\sigma}\} \equiv \{..., \sigma_{s-2}, \sigma_{s+2}, ...\}$. For this, we define a reduced probability

$$p(\sigma_{s-1}, \sigma_s, \sigma_{s+1}) \equiv \sum_{\{\bar{\sigma}\}} P(\{\sigma\}) \tag{45}$$

so that the sum

$$\mathcal{K}(\sigma_s \to -\sigma_s|\sigma_{s-1}, \sigma_{s+1}) \equiv \sum_{\{\bar{\sigma}\}} K^*(\{\sigma\} \to \mathcal{F}_s\{\sigma\})$$

is simply

$$\frac{w_0}{2}\left[1 - \gamma_s\sigma_s\frac{\sigma_{s-1} + \sigma_{s+1}}{2}\right]p(\sigma_{s-1}, \sigma_s, \sigma_{s+1}) - \frac{w_0}{2}\left[1 + \gamma_s\sigma_s\frac{\sigma_{s-1} + \sigma_{s+1}}{2}\right]p(\sigma_{s-1}, -\sigma_s, \sigma_{s+1})$$

From (44), it is easy to show that, in the $L \to \infty$ limit (where $\lambda^L \to 0$),

$$p(\sigma_{s-1}, \sigma_s, \sigma_{s+1}) \to \frac{1}{2}\sum_{\tau_s}\left[\frac{1 + \lambda h_{s-1}\tau_s\sigma_{s-1}}{2}\right]\left[\frac{1 + h_s\tau_s\sigma_s}{2}\right]\left[\frac{1 + \lambda h_{s+1}\tau_s\sigma_{s+1}}{2}\right]$$

$$= \frac{1}{8}\left[1 + \lambda h_e h_o(\sigma_{s-1} + \sigma_{s+1})\sigma_s + (\lambda h_{s-1})^2\sigma_{s-1}\sigma_{s+1}\right]$$

where we have used $h_{s-1} = h_{s+1}$ and $h_{s-1}h_s = h_e h_o$. As a result,

$$\mathcal{K}(\sigma_s \to -\sigma_s|\sigma_{s-1}, \sigma_{s+1}) \to \frac{w_0}{8}\left[2\lambda h_e h_o - \gamma_s\left(1 + \lambda^2 h_{s-1}^2\right)\right]\{\sigma_s(\sigma_{s-1} + \sigma_{s+1})/2\}.$$

Note that the last factor assumes the values $\pm 1, 0$ only. After some algebra, we find a particularly simple result:

$$|\mathcal{K}(\sigma_s \to -\sigma_s|\sigma_{s-1}, \sigma_{s+1})| = \begin{cases} |\gamma_e - \gamma_o|(w_0/16) & \text{for} \quad \sigma_{s-1} = \sigma_{s+1} \\ 0 & \text{for} \quad \sigma_{s-1} \neq \sigma_{s+1} \end{cases} \tag{46}$$

Note that this current *sum* vanishes for $\sigma_{s-1} \neq \sigma_{s+1}$, even though individual currents may be non-zero. Such a result is not surprising, given that the sum restores an

underlying up-down symmetry. Finally, we remark that all quantities for finite L are available, and this expression turns out to be *exact* for any L. Details of these findings, as well as extensions such as computing current *loops,* will be published elsewhere [36].

We end this subsection by illustrating how the currents can be used for computing fluxes. In particular, we recover the results of [21] concerning the energy flow into/out of the spin chain from the bath with the higher/lower temperature. When one spin (say, σ_s) is flipped, the energy change in the system is just

$$\Delta\mathcal{H}\left(\sigma_s \to -\sigma_s\right) = 2J\sigma_s\left(\sigma_{s-1} + \sigma_{s+1}\right).$$

Since this change is independent of all the other spins, we can simply multiply it with $\mathcal{K}\left(\sigma_s \to -\sigma_s\right)$ to obtain the rate of *net* change (in the steady state). The result is $w_0 J\left(\gamma_{s-1} - \gamma_s\right)\left(\sigma_{s-1} + \sigma_{s+1}\right)^2/8$, so that the configurational average is $w_0 J\left(\gamma_{s-1} - \gamma_s\right)$. Note that, if $T_s > T_{s-1}$, then $\gamma_{s-1} > \gamma_s$ so that there is an average energy flow "into" the system due to flipping the spin at site s. Thus, the net flux *through* our system is $w_0 J\left|\gamma_{s-1} - \gamma_s\right|/2$, a result phrased as "the energy flow from an even to an odd site" in [21]. Interestingly, these energy fluxes are directly related to the entropy production [22, 21].

5.4. NESS Gaussian distributions

Another exactly solvable system is $\mathcal{N}$ "particles" (or simply, degrees of freedom), subjected to linear forces (e.g., generalized coupled harmonic oscillators) and Gaussian noise. Although the configuration space of this system is continuous, it is sufficiently simple that both P^* and K^* are explicitly known, serving as an elegant illustration of our formalism. It can be regarded as the continuum limit of a particular biased random walk on, say, a hypercubic lattice. Specifically, the jump rates have a bias which depends linearly on the location of the walker from the origin *and* may be anisotropic.

We begin with a Langevin equation for the degrees of freedom ("coordinates") ξ^μ ($\mu = 1, ..., \mathcal{N}$) and the associated Fokker-Planck equation for $P\left(\vec{\xi}, t\right)$. The latter is the master equation for this system, with a stationary distribution known to be Gaussian. If detailed balance is violated, the stationary probability currents can nevertheless be computed. This subsection will be devoted to the highlights, with details left to Appendix D. In this spirit, we will use a compact notation of vectors (e.g., $\vec{\xi}$) and matrices (blackboard bold font) here, while in Appendix D, all indices will be explicitly displayed.

Consider a Langevin equation with linear deterministic forces:

$$\partial_t \vec{\xi}\left(t\right) = -\mathbb{F}\vec{\xi}\left(t\right) + \vec{\eta}\left(t\right) \tag{47}$$

and Gaussian noise (uncorrelated in time):

$$\begin{aligned} \langle\vec{\eta}\left(t\right)\rangle &= 0 \\ \langle\vec{\eta}\left(t\right) \otimes \vec{\eta}\left(t'\right)\rangle &= \mathbb{N}\delta\left(t - t'\right). \end{aligned}$$

Here, $\mathbb{F}$ is an arbitrary real matrix, except that, for stability and to model dissipation, the real part of its spectrum must be positive. We denote the eigenvalues and the right and left eigenvectors of F by

$$\mathbb{F}\vec{u}_I = \lambda_I \vec{u}_I \quad \text{and} \quad \vec{v}_I \mathbb{F} = \lambda_I \vec{v}_I \tag{48}$$

with $\operatorname{Re}\lambda_I > 0$, and $I = 1, 2, ..., \mathcal{N}$. Meanwhile, the noise matrix $\mathbb{N}$ must clearly be real symmetric, as well as positive. For example, if the discrete random walker has anisotropic jump rates, then $\mathbb{N}$ is diagonal but not proportional to the unit matrix.

The associated Fokker-Planck equation reads

$$\partial_t P\left(\vec{\xi}, t\right) = \vec{\nabla} \cdot \left\{ \frac{\mathbb{N}}{2} \vec{\nabla} + \mathbb{F}\vec{\xi} \right\} P\left(\vec{\xi}, t\right) \tag{49}$$

with the probability currents

$$\vec{K} \equiv - \left\{ \frac{\mathbb{N}}{2} \vec{\nabla} + \mathbb{F}\vec{\xi} \right\} P\left(\vec{\xi}, t\right). \tag{50}$$

If the matrices $\mathbb{N}$ and $\mathbb{F}$ are constrained such that $\mathbb{N}^{-1}\mathbb{F}$ is *symmetric*, then we can define

$$\mathbb{V} \equiv 2k_B T \mathbb{N}^{-1}\mathbb{F} \tag{51}$$

and see that this is just a system of coupled simple harmonic oscillators, subjected to (a general Gaussian) noise. Such a system will settle into thermal equilibrium, with the familiar Boltzmann distribution:

$$P^{eq}\left(\vec{\xi}\right) \propto \exp\left\{ -\frac{\vec{\xi}\mathbb{V}\vec{\xi}}{2k_B T} \right\}$$

as well as a trivially vanishing $\vec{K}$. Of course, Equation (51) with *symmetric* $\mathbb{V}$ is just the detailed balance condition here and expresses the usual fluctuation-dissipation relation.

However, if we insist on studying the general case where $\mathbb{N}^{-1}\mathbb{F}$ is *not* symmetric, we will encounter a NESS with non-trivial $\vec{K}$'s. (For $\mathcal{N} = 3$, we would write such a $\vec{K}$ as *curl* of some vector field.) To see this explicitly, we recognize that the stationary distribution is still a Gaussian [37]

$$P^*\left(\vec{\xi}\right) \propto \exp\left[-\frac{\vec{\xi}\mathbb{C}^{-1}\vec{\xi}}{2} \right], \tag{52}$$

where $\mathbb{C}$ is the correlation matrix:

$$\left\langle \vec{\xi} \otimes \vec{\xi} \right\rangle = \mathbb{C}. \tag{53}$$

To find $\mathbb{C}$ in terms of $\mathbb{N}$ and $\mathbb{F}$ is straightforward, but not trivial (Appendix D). A convenient expression is:

$$\mathbb{C} = \sum_{I,J} \frac{\langle \vec{v}_I \mathbb{N} \vec{v}_J \rangle}{\lambda_I + \lambda_J} \vec{u}_I \otimes \vec{u}_J, \tag{54}$$

which is manifestly symmetric.

Turning to the stationary currents, we see that the second term in

$$\vec{K}^* \equiv -\left\{\frac{\mathbb{N}}{2}\vec{\nabla} + \mathbb{F}\vec{\xi}\right\} P^*\left(\vec{\xi}\right) \tag{55}$$

can be written as $-\mathbb{FC}\vec{\nabla}P^*$. Thus, $\vec{K}^* \equiv \{\mathbb{FC} - \mathbb{N}/2\}\vec{\nabla}P^*$. To see that $\mathbb{FC} - \mathbb{N}/2$ is indeed *antisymmetric* (so that $\vec{\nabla}\cdot\vec{K}^* = 0$), we only need to recall that $\vec{u}_I$ are eigenvectors of $\mathbb{F}$, so that

$$\mathbb{FC} = \sum_{I,J} \frac{\langle \vec{v}_I \mathbb{N} \vec{v}_J \rangle}{\lambda_I + \lambda_J} \lambda_I \vec{u}_I \otimes \vec{u}_J \ .$$

The final result is quite simple:

$$\vec{K}^* = \mathbb{A}\vec{\nabla}P^* \ , \tag{56}$$

where

$$\mathbb{A} \equiv \frac{1}{2} \sum_{I,J} \frac{\lambda_I - \lambda_J}{\lambda_I + \lambda_J} \langle \vec{v}_I \mathbb{N} \vec{v}_J \rangle \, \vec{u}_I \otimes \vec{u}_J \tag{57}$$

is manifestly antisymmetric. Of course, we can evaluate the gradient in Equation (56) explicitly, with the result

$$\vec{K}^* = -\left(\mathbb{A}\mathbb{C}^{-1}\vec{\xi}\right) P^* \ . \tag{58}$$

One interesting consequence is that the expression in Equation (17) can be neatly evaluated:

$$\int \left|\vec{K}^*\right|^2 = \frac{1}{2}Tr\left\{\mathbb{A}\mathbb{C}^{-1}\mathbb{A}^\top\right\} \ .$$

Lastly, let us consider "generalized detailed balance": What is the class of dynamics that will lead us to a given NESS, i.e., $\{P^*, K^*\}$ or more specifically in this case, $\{\mathbb{C}, \mathbb{A}\}$? Since the configuration space here is not finite, it does not seem trivial to provide the *entire* class of allowable dynamics. However, since we know P^* explicitly, we can exploit Equation (27) and add $\int d\vec{\xi}' \left\{\Delta(\vec{\xi}, \vec{\xi}')P(\vec{\xi}', t) - \Delta(\vec{\xi}', \vec{\xi})P(\vec{\xi}, t)\right\}$ to the right hand side of Equation (49), where $\Delta\left(\vec{\xi}, \vec{\xi}'\right)$ is *any function* that is non-negative and satisfies

$$\frac{\Delta\left(\vec{\xi}, \vec{\xi}'\right)}{\Delta\left(\vec{\xi}', \vec{\xi}\right)} = \exp\left\{\frac{\vec{\xi}'\mathbb{C}^{-1}\vec{\xi}' - \vec{\xi}\mathbb{C}^{-1}\vec{\xi}}{2}\right\} \ .$$

Unfortunately, this expression is too general to be illuminating. To provide some insight, let us illustrate this freedom by studying a small subset of the allowable modifications. Let us frame this question as the "inverse" of the usual one. Ordinarily, we are *given* the matrices $\{\mathbb{F}, \mathbb{N}\}$, and are asked to find the NESS (in this case, $\{\mathbb{C}, \mathbb{A}\}$). The inverse question is: Given $\{\mathbb{C}, \mathbb{A}\}$, what can be said about $\{\mathbb{F}, \mathbb{N}\}$, i.e., what dynamics will insure that we arrive at the above $\{P^*, K^*\}$? Clearly, the key equation is just $\mathbb{FC} - \mathbb{N}/2 = \mathbb{A}$. Specifically, we are allowed to choose *any* $\mathbb{N}$, provided it is a valid

noise correlation (real, symmetric, positive matrix) and construct the dissipative forces $\mathbb{F}$ according to

$$\mathbb{F} = \mathbb{C}^{-1} \left\{ \mathbb{N}/2 + \mathbb{A} \right\} . \tag{59}$$

It may also appears as if we can choose any matrix $\mathbb{F}$ and simply compute $\mathbb{N}$ from

$$\mathbb{N} = 2 \left\{ \mathbb{F}\mathbb{C} - \mathbb{A} \right\} . \tag{60}$$

A closer examination reveals a difficulty with this naive approach. For fixed $\{\mathbb{C}, \mathbb{A}\}$, not every choice of $\mathbb{F}$ will lead to a *symmetric* $\mathbb{N}$ (a necessary condition for the noise correlation)! This issue is related to the discussion of Equation (51).

We end this subsection with two comments. The concerned reader may ask: Why can we choose an arbitrary $\mathbb{N}$ but not any $\mathbb{F}$? The difference lies in that $\mathbb{N}$ has fewer parameters than $\mathbb{F}$. There is an intimate connection to the general case where only the symmetric part of $\bar{W}_i^j$ can be chosen freely. Since $\mathbb{N}$ must be symmetric, it evidently contains all the freedom of choice available (in this subclass of dynamics). By contrast, $\mathbb{F}$ appears to have no particular symmetry; yet the antisymmetric part of $\mathbb{C}\mathbb{F}$ is completely fixed (by $\mathbb{A}$). Finally, to make contact with ordinary detailed balance, it is easier to consider Equation (60) and follow how it reduces for the textbook case of an equilibrium system with the most trivial dynamics: We have (i) a Hamiltonian $\mathcal{H} = \vec{\xi}\mathbb{V}\vec{\xi}/2$; (ii) forces $\kappa \left(-\vec{\nabla}\mathcal{H} \right)$ where κ is a dissipative coefficient; and (iii) $\mathbb{C} = (\mathbb{V}/k_B T)^{-1}$. Thus, $\mathbb{A} \equiv 0$; and $\mathbb{N} = 2\mathbb{F}\mathbb{C}$ is just $2\kappa k_B T \times$ the unit matrix.

6. Summary and Outlook

In this paper, we propose that a *non-equilibrium* steady state be characterized not only by $P^*(\mathcal{C})$, the stationary distribution for finding the system in configuration $\mathcal{C}$, but also $K^*(\mathcal{C}, \mathcal{C}')$, the *net* probability current from $\mathcal{C}$ to $\mathcal{C}'$. The pair $\{P^*, K^*\}$ forms a natural generalization of having P^{eq} as the quantity that characterizes all details of an equilibrium state. Within the context of a master equation approach, in which the dynamics of a system is defined by a set of transition rates $w(\mathcal{C} \to \mathcal{C}')$, we recalled a graphic method for constructing the pair $\{P^*, K^*\}$, as well as the intimate relationship between K^* and irreversible cycles associated with the rates. Assuming ergodic rates, this steady state is unique.

Exploring the consequences of our postulate, we find that the converse - finding a set of w's which leads to a given $\{P^*, K^*\}$ - is far from unique: The rates are only bound by a certain set of constraints. This condition is well known, to those who study *equilibrium* systems by computer simulations, as "detailed balance:"

$$w(\mathcal{C} \to \mathcal{C}') P^{eq}(\mathcal{C}) - w(\mathcal{C}' \to \mathcal{C}) P^{eq}(\mathcal{C}') = 0$$

The proposed generalization to *non*-equilibrium systems is almost intuitive, namely,

$$w(\mathcal{C} \to \mathcal{C}') P^*(\mathcal{C}) - w(\mathcal{C}' \to \mathcal{C}) P^*(\mathcal{C}') = K^*(\mathcal{C}, \mathcal{C}') .$$

Since the only difference between this and the equilibrium condition is the value of the right hand side, we are "just as free" in choosing rates in either case. In

other words, the equivalence classes of rates are the same, except for one subtlety explained in Section 4. A unified way of making this statement is the following. Two sets of rates belong to the same class provided their *differences,* $\Delta\left(\mathcal{C}\to\mathcal{C}'\right)$, satisfy $\Delta\left(\mathcal{C}\to\mathcal{C}'\right)P^{*}\left(\mathcal{C}\right)=\Delta\left(\mathcal{C}'\to\mathcal{C}\right)P^{*}\left(\mathcal{C}'\right)$. A further consequence of these degrees of freedom is that the entropy production (associated with the reservoirs coupled to our system, driving it to a NESS [13]) can be made infinitesimally small or arbitrarily large. We also proposed that $\Sigma\left(K^{*}\right)^{2}$ can be exploited to measure of how "far" a NESS is away from equilibrium. Of course, it would be better if a *dimensionless* quantity could be identified, so that common phrases like "systems far from equilibrium" can be given a universal and quantitative meaning. Finally, a number of examples were presented, illustrating these ideas.

While we hope that this work provides a fresh perspective on non-equilibrium steady states, we are aware of much room for improvements and further investigations. Let us end with a brief outlook.

For simplicity, we focused mainly on a master equation with continuous time and discrete configuration space. Generalizations to systems with continuous configuration space should be possible, though there may be non-trivial mathematical obstacles. We believe that the example in 5.4 represents a possible starting point. The more general case is the Fokker-Planck equation, which admits transitions between configurations $\{\phi\left(\vec{x}\right)\}$ that are infinitesimally close: $\delta\phi\left(\vec{x}\right)$. Much work has been devoted to this equation for NESS [38], and the resulting conclusions should be exploited. On a different note, formulations involving discrete time present a different challenge. Since the transition "rates" are now conditional probabilities, their proper normalization will lead to further constraints on the choice of w's, beyond those listed in Section 4) . However, we anticipate this complication to be minor.

As more serious question, yet to be answered for arbitrary NESS's, is the existence and uniqueness of thermodynamic limits. For example, there is a belief that, for the driven Ising lattice gas in two dimensions, different steady states will be reached in this limit, depending on the aspect ratio of the system [39]. Perhaps devoting some attention to the distribution of probability currents will facilitate this quest. This topic is also intimately related to the issue of the "micro-macro connection." Starting as a vague notion of "coarse graining," this connection has gained much substance through the renormalization group (RG), especially in the study of critical phenomena. For systems in equilibrium, the distribution (P^{eq}) is uniquely linked to a Hamiltonian ($\mathcal{H}$) by the Boltzmann factor, and the progression from a microscopic, via a mesoscopic, to a macroscopic description can be cast in the language of RG flows in the space of $\mathcal{H}$'s or P's. We believe that, for NESS, the flow in the space of K^{*}'s will play an equally important role, on a par with the flow of P^{*}. To illustrate this thought, let us highlight two seemingly similar NESS systems in which the RG flows end at very different types of fixed points. Specifically, for the uniformly driven Ising lattice gas [33], the RG fixed point is a "genuinely non-equilibrium" dynamic functional [40] which *cannot* be written in the form of any equilibrium system with an $\mathcal{H}$. By contrast, if the same system is

driven randomly, the fixed point corresponds to an equilibrium uniaxial system with dipolar interactions [41]. This example suggests that the RG flow of K^* leads to some non-trivial fixed point in one case and, in the other case, ends at the "trivial" fixed point $K^* = 0$. One hint from physics is that there are global (particle) currents in the first system, which cannot vanish under the RG. In contrast, non-trivial microscopic probability currents in the second system are most likely local, so that they vanish under RG transformations. Work is in progress to provide solid foundations for these promising notions.

Entropy production is another venerable issue. Through its coupling to more than one energy reservoir, our system can be regarded as an agent which redistributes energy from one or more of these reservoirs to the rest. The most intuitive and simple example is given in Section 5.3 above - an Ising model coupled to two thermals baths at different temperatures. Heat flows from the hotter bath into the spin system and then to the cooler bath. In the steady state, all thermodynamic quantities of the Ising system are constant on the average, including this heat *through-flux*. Thus, there is a constant rate of energy redistribution associated with "the environment" (or "the medium"), a term we use to refer to the totality of *all* the external reservoirs. Associated with this energy redistribution should be an entropy production of the environment. In general, given the detailed dynamics of the environment and how it couples to our system, it is possible, in principle, to compute this rate of entropy production. However, in our framework, we start with a master equation. Expressed in terms of transition rates, it captures the dynamics of the system and how the system couples to the environment, but carries no information about the dynamics of the latter. As a result, it is not clear how we can unambiguously find the rate of entropy production of the medium. Nevertheless, it seems possible to define an entropy production, associated with the system-medium *coupling*. Relying on the context of chemical reactions, Schnakenberg proposed such a definition, which depends only on the w's in the master equation. Thus, it is a natural candidate for us to exploit here (see Section 4.2), even though its relation to the true entropy production of the medium is not definitive. There may be other, better grounded, definitions [42]. We believe it will be worthwhile exploring them also in the context of K^*. In a related vein, we mention fluctuation-dissipation and work-energy theorems associated with NESS [43]. Apart from considerable theoretical interests over the last two decades, recent experimental measurements in a variety of systems have contributed to the excitement focused on these issues [44]. Whether the probability currents provide novel insight here deserves to be studied.

Finally, let us return to the analogy with electrodynamics, in which a parallel is drawn between electrostatics/magnetostatics and equilibrium/non-equilibrium steady states. Of course, we are aware of considerable conceptual difficulties, especially for the general case where transitions between all configurations are allowed. However, for cases with a local dynamics (e.g., Glauber spin flips for an Ising model or a Fokker-Planck equation in continuous configuration space), an induced metric can be defined [45] so that the probability current is just a vector field. Since K^* is divergence-free, it can

be expressed as a (generalized) curl of a vector potential and 'magnetic fields' can also be defined [45]. It behooves us to ask whether such fields might be meaningful, and if their properties can be exploited. Pursuing this parallel with electrodynamics far into the future, we may seek an underlying gauge theory [46] and see if it might provide a unified description of all time-dependent phenomena in statistical mechanics.

The comments above highlight just a few of the issues surrounding the central quest: providing a sound framework for the statistical mechanics of non-equilibrium steady states, on a par with the Boltzmann-Gibbs approach for equilibrium systems. We hope that our proposal - to bring the microscopic probability current distribution, K^*, onto center stage, as an equal partner with the microscopic distribution of probabilities, P^* - will generate further explorations and discussions in the pursuit of our quest.

Acknowledgments

Appendix A. Kirchhoff's problem and its relation to NESS

In most expositions of the graphic approach to finding the stationary distribution from the master equation, Kirchhoff's solution [15] to the electrical network problem is referenced. Here, we offer some comparisons and contrasts.

At first glance, it appears that both problems have the same underlying network structure (N vertices and $N(N-1)/2$ edges) and the same number of parameters: $2 \times N(N-1)/2$. For electrical networks, Kirchhoff [15] posed a resistance (R_{ij}) and an electromotive force ($\mathcal{E}_{ij}$) between the nodes i and j. The former/latter are strictly symmetric/antisymmetric. Naively, since we have w_i^j (with $i \neq j$), we may think of identifying the symmetric and antisymmetric parts of w with R and $\mathcal{E}$, and perhaps formulate an exact mapping between the two problems.

On closer examination, differences emerge. To seek the NESS, we need to solve N equations for N unknowns (P_i^*). No other equations need be solved to obtain the $N(N-1)/2$ currents; they are just linear combinations of the P^*'s. By contrast, by focusing on the currents (I_{ij}, also antisymmetric) as the unknowns, Kirchhoff needed far more equations. In his paper, there are N equations for the nodes:

$$\sum_j I_{ij} = 0$$

for each i, and $N(N-3)/2 + 1$ equations for the loops:

$$\mathcal{E}_{k_1 k_2} + ... + \mathcal{E}_{k_n k_1} - R_{k_1 k_2} I_{k_1 k_2} ... - R_{k_n k_1} I_{k_n k_1} = 0 \ .$$

Of course, we recognize that the node equations correspond to the master equation for the steady state and that loop equations allow us to define a single-valued function associated with each node. Traditionally, this is called the "potential," V_i, which can be defined through the differences

$$V_i - V_j \equiv \mathcal{E}_{ij} - R_{ij}I_{ij} \ .$$

Clearly this is not the only possible definition of the single-valued function, since any well-behaved function of V_i will produce another single-valued function. Even if we demand linearity between V and I, the above is unique only up to two parameters: a constant shift and an overall scale: $V \rightarrow \lambda\left(V - v\right)$. If we were to try to identify P_i^* with the potential, we will need the shift to insure positivity (since potentials can easily be negative) and the scale for normalization of P^*. But the shift is arbitrary (apart from a lower bound), so that the ratios $\left(V_i - v\right)/\left(V_j - v\right)$ are not fixed. In this sense, there is no way to generate a unique quantity like P_i^* from the currents of the Kirchhoff problem.

Forcing the issue from the other direction seems more feasible, since there is no problem choosing the potentials V_i to be P_i^*. From the definition $K^{*j}_{\ \ i} \equiv w_i^j P_j^* - w_j^i P_i^*$, we can write

$$P_i^* = \frac{w_i^j}{w_j^i}P_j^* + \frac{1}{w_j^i}K^{*j}_{\ \ i}$$

Formally, we can substitute the expression in Equation (10) for P_j^* and write the first term ($w_i^j P_j^*/w_j^i$) as $G_i^j\left[\{w\}\right]$. Then, we have

$$P_i^* - P_j^* = \left[G_i^j - G_j^i\right] - \left[\frac{1}{w_j^i} + \frac{1}{w_i^j}\right]K^{*i}_{\ \ j} \ .$$

Taken at face value, we can exploit this equation to identify

$$\begin{aligned}
P_i^* &\rightarrow V_i \\
K^{*i}_{\ \ j} &\rightarrow I_{ij} \\
G_i^j - G_j^i &\rightarrow \mathcal{E}_{ij} \\
\frac{1}{w_j^i} + \frac{1}{w_i^j} &\rightarrow R_{ij}
\end{aligned}$$

The lack of a one-to-one mapping between $\{R, \mathcal{E}\}$ and $\{w\}$ can now be summarized succinctly. From the former, we can find a unique solution for the currents, but not the charges (or potentials). Even if we could and these were identified with K^* and P^*, we know that there is a whole class of w's which leads to the very same $\{P^*, K^*\}$. Finally, in passing, we mention that there are intimate connections between Kirchhoff's problem and the percolation problem. Details may be found in the context of an extensive review on the Potts model [47].

Appendix B. A maximally asymmetric $N = 4$ example: TASEP with two sites

For a totally asymmetric exclusion process (TASEP) on a one-dimensional chain with open boundaries [17, 18] with two sites, we show all the configurations in Figure 4. From the transition matrix, Equation (34), we see that there are only 5 non-zero arrows in the full space, shown in Figure 5(a). As a result, there are very few non-trivial directed trees. In Figure 5(b), we show the only tree directed towards vertex 1 that is non-zero. For vertex 3, there are two trees, shown in Figure 5(c) and (d). Thus, we arrive at, respectively, $P^*_{1,2,3,4} \propto \beta\gamma\beta, \alpha\beta\gamma, \alpha\alpha\beta + \beta\beta\alpha, \alpha\gamma\alpha$, and $\mathcal{Z}$ in Equation (10) is just $\alpha^2\beta + \beta^2\alpha + (\alpha^2 + \alpha\beta + \beta^2)\gamma$. To illustrate Equation (14), we consider, e.g., K^{*1}_3 which is β/Z. In graphic terms, we add a down arrow from vertex 1 to 3 to Figure 5(b), forming an irreversible loop associated with $\Pi[\mathcal{L}] = \alpha\beta\gamma$. Meanwhile, there is only one side branch, so that $R = \beta$ here. Thus, $K^{*1}_3 = \Pi R/\mathcal{Z} = \alpha\beta\gamma\beta/(\alpha\beta\gamma Z)$, in agreement with the above.

From these K^*'s, we can evaluate the particle current flowing into the system. Referring to Equation (20), it is clear that we just need to consider $(1 - n_1)n'_1$, which is zero for all configuration pairs, *except* being unity for the $(1, 3)$ and $(2, 4)$ pairs. Thus,

$$\langle J^* \rangle = K^{*1}_3 + K^{*2}_4 = (\alpha + \beta)/Z .$$

In steady state, it is clear that this expression will also equal the current flowing between the two sites: K^{*3}_2, or out of the system: $K^{*2}_1 + K^{*4}_3$.

Next, we turn to the dynamic equivalence classes associated with this W. We first compute the matrix $\bar{W}$, and then extract its symmetric and its antisymmetric part, resulting in:

$$S = \frac{1}{2}Z^{-1} \begin{pmatrix} -2\beta & \beta & \beta & 0 \\ \beta & -2(\alpha + \beta) & \alpha + \beta & \alpha \\ \beta & \alpha + \beta & -2(\alpha + \beta) & \alpha \\ 0 & \alpha & \alpha & -2\alpha \end{pmatrix} \tag{B.1}$$

$$A = \frac{1}{2}Z^{-1} \begin{pmatrix} 0 & \beta & -\beta & 0 \\ -\beta & 0 & \alpha + \beta & -\alpha \\ \beta & -(\alpha + \beta) & 0 & \alpha \\ 0 & \alpha & -\alpha & 0 \end{pmatrix} \tag{B.2}$$

We clearly recognize the values of the K^*'s in the elements of A.

Since S is a 4×4 symmetric matrix with constrained diagonal elements, we have 6 degrees of freedom. Selecting just one of these, for the purposes of illustration, we can define a new matrix, $\hat{S}$, by, e.g., modifying the $(3, 2)$ and $(2, 3)$ elements by an amount 2ϵ, and preserving the column sums

$$\hat{S} = \frac{1}{2}Z^{-1} \begin{pmatrix} -2\beta & \beta & \beta & 0 \\ \beta & -2(\alpha + \beta) - 2\epsilon & \alpha + \beta + 2\epsilon & \alpha \\ \beta & \alpha + \beta + 2\epsilon & -2(\alpha + \beta) - 2\epsilon & \alpha \\ 0 & \alpha & \alpha & -2\alpha \end{pmatrix}$$

Respecting the symmetries and the constraint (25), the new rate matrix $\hat{W}$ is given by

$$\hat{W} = \left[\hat{S}_i^j + \frac{1}{2} K^{*j}_i \right] (P_j^*)^{-1} = \begin{pmatrix} -\alpha & \beta & 0 & 0 \\ 0 & -(\alpha+\beta) - \epsilon & \gamma + \frac{\gamma}{\alpha+\beta}\epsilon & 0 \\ \alpha & \epsilon & -(\alpha+\beta) - \frac{\gamma}{\alpha+\beta}\epsilon & \beta \\ 0 & \alpha & 0 & -\beta \end{pmatrix}$$

Comparing to the original matrix W, we can see that the new feature is a transition from configuration 2 to 3 which was absent in the original model. In other words, the particle is now allowed to jump backwards. The matrix Δ is nonzero only in the 2×2 submatrix involving configurations 2 and 3:

$$\Delta \equiv \hat{W} - W = \epsilon \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & -1 & \frac{\gamma}{\alpha+\beta} & 0 \\ 0 & 1 & -\frac{\gamma}{\alpha+\beta} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

It is easy to check that it satisfies Equation (27).

Let us now recalculate the particle current from the first to the second site, keeping in mind that the particle can now also jump backwards. However, the probability current between configurations 2 and 3 is unchanged, as one can see from a quick explicit check:

$$K^{*3}_{\ 2} = \hat{w}_2^3 P_3^* - \hat{w}_3^2 P_2^* = Z^{-1} \left[\left(\gamma + \frac{\gamma}{\alpha+\beta}\epsilon \right) \frac{(\alpha+\beta)}{\gamma} - \epsilon \right] = Z^{-1} (\alpha + \beta)$$

Since each term in the equation above is associated with a single particle hop, it is immediately obvious that $\langle J^* \rangle$ also remains invariant, under the transformation from W to $\hat{W}$.

Allowing for backwards hops of the particle may appear rather innocuous. A more drastic modification would be to allow transitions between configurations 1 and 4 which are completely absent in the original model. This leads to

$$\hat{S} = \frac{1}{2} Z^{-1} \begin{pmatrix} -2(\beta+\epsilon) & \beta & \beta & 2\epsilon \\ \beta & -2(\alpha+\beta) & \alpha+\beta & \alpha \\ \beta & \alpha+\beta & -2(\alpha+\beta) & \alpha \\ 2\epsilon & \alpha & \alpha & -2(\alpha+\epsilon) \end{pmatrix}$$

and

$$\hat{W} = W + \epsilon \begin{pmatrix} -\alpha/\beta & 0 & 0 & \beta/\alpha \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \alpha/\beta & 0 & 0 & -\beta/\alpha \end{pmatrix}$$

Again, the difference between the two sets of rates satisfies detailed balance with respect to P^*. As a result, the probability current $K^{*1}_{\ 4}$, associated with transitions between configurations 1 and 4, remains zero. This also ensures that the physical current, $\langle J^* \rangle$, remains unaffected.

Since all of these rates involve at least one uni-directional transition, they are all associated with infinite entropy production. In order to obtain a finite value for the

entropy production, we need to start from a rate matrix where each forward transition is associated with a backward one. Starting from the original W and its associated S, Equation (B.1), and recalling that we have 6 degrees of freedom, parameterized by ϵ_1, $\epsilon_2, ..., \epsilon_6$, the most general $\hat{S}$ would be

$$\hat{S} = S + Z^{-1}\begin{pmatrix} -(\epsilon_1 + \epsilon_2 + \epsilon_3) & \epsilon_1 & \epsilon_2 & \epsilon_3 \\ \epsilon_1 & -(\epsilon_1 + \epsilon_4 + \epsilon_5) & \epsilon_4 & \epsilon_5 \\ \epsilon_2 & \epsilon_4 & -(\epsilon_2 + \epsilon_4 + \epsilon_6) & \epsilon_6 \\ \epsilon_3 & \epsilon_5 & \epsilon_6 & -(\epsilon_3 + \epsilon_5 + \epsilon_6) \end{pmatrix}$$

The associated $\hat{W}$ is given by

$$\hat{W} = W + \begin{pmatrix} -(\epsilon_1 + \epsilon_2 + \epsilon_3)\frac{\alpha}{\beta} & \epsilon_1 & \epsilon_2\frac{\gamma}{\alpha+\beta} & \epsilon_3\frac{\beta}{\alpha} \\ \epsilon_1\frac{\alpha}{\beta} & -(\epsilon_1 + \epsilon_4 + \epsilon_5) & \epsilon_4\frac{\gamma}{\alpha+\beta} & \epsilon_5\frac{\beta}{\alpha} \\ \epsilon_2\frac{\alpha}{\beta} & \epsilon_4 & -(\epsilon_2 + \epsilon_4 + \epsilon_6)\frac{\gamma}{\alpha+\beta} & \epsilon_6\frac{\beta}{\alpha} \\ \epsilon_3\frac{\alpha}{\beta} & \epsilon_5 & \epsilon_6\frac{\gamma}{\alpha+\beta} & -(\epsilon_3 + \epsilon_5 + \epsilon_6)\frac{\beta}{\alpha} \end{pmatrix}$$

Evaluating the entropy production for this general form, we arrive at

$$\dot{\mathbf{S}}^*_{tot} = \frac{1}{2}\sum_{i,j} K^{*j}_i \ln \frac{W^j_i P^*_j}{W^i_j P^*_i} = \frac{1}{2}\sum_{i,j} K^{*j}_i \ln \frac{S^j_i + A^j_i}{S^j_i - A^j_i}$$

$$= Z^{-1}\left\{ \beta\ln\frac{\beta + \epsilon_1}{\epsilon_1} + \beta\ln\frac{\beta + \epsilon_2}{\epsilon_2} + (\alpha + \beta)\ln\frac{\alpha + \beta + \epsilon_4}{\epsilon_4} \right.$$

$$\left. +\alpha\ln\frac{\alpha + \epsilon_5}{\epsilon_5} + \alpha\ln\frac{\alpha + \epsilon_6}{\epsilon_6} \right\}$$

which is clearly finite now.

Appendix C. Currents in generalized mass transport models

Here, we provide a further example associated with mass transport models, namely, the generalization from discrete to continuous masses, with parallel updates in discrete time. Thus, we consider a ring of discrete sites occupied by *continuous* m_s's. The evolution proceeds in discrete time steps, with μ_s being chipped off from m_s and added to m_{s+1}, for all sites at once. To distinguish the conditional probability here from the case in the main text, we denote it by $\phi(\mu|m)$ here. Though the fundamental issues for this non-equilibrium process and the one with continuous time and random sequential updates are the same, there are a few differences, on which we will comment here.

As in the previous case, P^* is known for a wide class of such models[29]: If $\phi(\mu|m)$ is of the form $v(\mu)u(m-\mu)/f(m)$ (where v and u are arbitrary non-negative functions, and $f(m) = \int v(\mu)u(m-\mu)\,d\mu$), then $P^*(\{m_s\}) = Z^{-1}\prod_s f(m_s)$, as in Section 5.2. Again, $w^j_i P^*_j$ in Equation (12) will assume the form $P^*(\{m_s\})w(\{m_s\} \to \{m'_s\})$. Unlike the random sequential case,

$$w(\{m_s\} \to \{m'_s\}) = \prod_s \phi(\mu_s|m_s)$$

so that *all* the f's cancel. Thus, we are left with a simple product:

$$P^* (\{m_s\}) \, w (\{m_s\} \to \{m'_s\}) = Z^{-1} \prod_s v (\mu_s) \, u (\sigma_s)$$

where μ_s (the mass to be moved) and σ_s (the remaining mass) are fixed by

$$\begin{aligned}
m_s &= \mu_s + \sigma_s \\
m'_s &= \mu_{s-1} + \sigma_s
\end{aligned} \tag{C.1}$$

Thus,

$$ZK^* (\{m_s\} \to \{m'_s\}) = \prod_s v (\mu_s) \, u (\sigma_s) - \prod_s v (\tilde{\mu}_s) \, u (\tilde{\sigma}_s) , \tag{C.2}$$

where $\tilde{\mu}_s$ and $\tilde{\sigma}_s$ satisfy $m'_s = \tilde{\mu}_s + \tilde{\sigma}_s$ and $m_s = \tilde{\mu}_{s-1} + \tilde{\sigma}_s$. Let us end with a few remarks.

First, it is clear that many different functions v and u will lead to the same convolution $f \equiv v * u$, so that all of them are associated with the same P^*. However, it is also clear that typically, K^* will *not* be the same. Thus, our framework provides a natural way to distinguish these different NESS's, all of which share the same stationary P^*.

Next, we should emphasize that this rather compact notation belies a subtlety: Starting with a pair of configurations $\{m_s, m'_s\}$, it is not possible in general to find a unique set $\{\mu_s, \sigma_s\}$. First, Equation (C.1), rewritten here as

$$\begin{aligned}
\mu_{s-1} + \sigma_s &= m'_s \\
\mu_s + \sigma_s \phantom{{}_{-1}} &= m_s
\end{aligned}$$

is just a simple linear equation of the form

$$\begin{pmatrix}
1 & 0 & \ldots & 0 & 1 \\
1 & 1 & \ldots & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
0 & 0 & \ldots & 1 & 0 \\
0 & 0 & \ldots & 1 & 1
\end{pmatrix}
\begin{pmatrix}
\sigma_1 \\
\mu_1 \\
\vdots \\
\sigma_L \\
\mu_L
\end{pmatrix}
=
\begin{pmatrix}
m'_1 \\
m_1 \\
\vdots \\
m'_L \\
m_L
\end{pmatrix}$$

Now, the matrix on the left has a zero eigenvalue and cannot, strictly, be inverted. However, the zero eigenvector ($+1/-1$ for even/odd elements) is associated with mass conservation. A physical set of $\{m_s, m'_s\}$ obeys $\sum_s (m_s - m'_s) = 0$ and has no component along this eigenvector. Thus, the existence of a solution is not in doubt.

In general, the solution is not unique, however. With parallel update, the transported masses $\{\mu_s, \sigma_s\}$ are determined by configurational masses $\{m_s, m'_s\}$ only up to an overall parameter $\bar{\mu}$. This extra "freedom" is associated with a simple physical process: The same configurational change can be achieved if we further chip off an identical amount, $\bar{\mu}$, from *all* sites and moved to the next, i.e., replacing $\{\mu_s, \sigma_s\}$ by $\{\mu_s + \bar{\mu}, \sigma_s - \bar{\mu}\}$. The range of allowed $\bar{\mu}$ is clear: None of the resultant μ's and σ's can be negative. Thus, if we start with any "minimal" set of μ_s's (i.e., at least one μ is zero), then the other sets can be generated by adding a positive $\bar{\mu}$, *provided* it is

no larger than the smallest m_s in the system. In other words, from any valid solution (i.e., non-negative $\{\mu_s, \sigma_s\}$) of Equation (C.1), $\bar{\mu}$ can decreased (or increased) until the smallest μ_s (or σ_s) vanishes. In this sense, we should integrate over this allowed range of $\bar{\mu}$ when computing the first term in the current in Equation (C.2).

Once a $\{\mu_s, \sigma_s\}$ solution is found, there is a simple way to construct the "complementary" set $\{\tilde{\mu}_s, \tilde{\sigma}_s\}$, which satisfies

$$\tilde{\mu}_{s-1} + \tilde{\sigma}_s = m_s$$
$$\tilde{\mu}_s + \tilde{\sigma}_s \quad = m_s'$$

Indeed, we can access the minimal set immediately. Let $\hat{\mu}$ be the largest of the μ's:

$$\hat{\mu} \equiv \sup \{\mu_s\}.$$

Then,

$$\tilde{\mu}_s = \hat{\mu} - \mu_s$$
$$\tilde{\sigma}_s = \sigma_s + \mu_s + \mu_{s-1} - \hat{\mu}.$$

Note that the one parameter family of allowed $\{\tilde{\mu}_s, \tilde{\sigma}_s\}$ is not necessarily the same as the one for $\{\mu_s, \sigma_s\}$. As a result, a different integral is needed here to compute the second term of K^* in Equation (C.2).

Appendix D. A simple example with continuous configuration space.

In the following, we provide the detailed analysis of the Langevin equation with linear deterministic forces (generalization of a system of coupled harmonic oscillators). The configuration space is $\mathcal{N}$-dimensional space: $\{\xi^\mu\}$ with $\mu = 1, ..., \mathcal{N}$. The Langevin equation for $\xi^\mu(t)$ reads:

$$\partial_t \xi^\mu = -F^\mu_\nu \xi^\nu + \eta^\mu$$

where F^μ_ν is an arbitrary real matrix, except that, for stability, the real part its spectrum must be positive (dissipative forces). The noise η is Gaussian with zero mean, i.e.,

$$\langle \eta^\mu(t) \rangle \quad\quad = 0$$
$$\langle \eta^\mu(t) \eta^\nu(t') \rangle = N^{\mu\nu} \delta(t - t')$$

where $N^{\mu\nu}$ is real symmetric and positive.

Let the eigenvalues and right/left eigenvectors of F be given by

$$\sum_\nu F^\mu_\nu u^\nu_I = \lambda(I) u^\mu_I; \quad \sum_\mu v^I_\mu F^\mu_\nu = \lambda(I) v^I_\nu$$
$$I \quad\quad = 1, ..., \mathcal{N}$$

with

$$\operatorname{Re} \lambda(I) > 0.$$

We choose eigenvectors so they form a complete bi-orthonormal set, i.e.,

$$\sum_I u^\nu_I v^I_\mu = \delta^\nu_\mu \quad\quad \sum_\mu v^I_\mu u^\mu_J = \delta^I_J.$$

The Fokker-Planck equation is

$$\partial_t P\left(\vec{\xi}, t\right) = \sum_{\mu, v} \left\{ \frac{1}{2} \partial_\mu N^{\mu\nu} \partial_\nu + \partial_\mu F_\nu^\mu \xi^\nu \right\} P\left(\vec{\xi}, t\right) \ , \tag{D.1}$$

where

$$\partial_\mu \equiv \frac{\partial}{\partial \xi_\mu}$$

differentiates all factors to its right.

The stationary distribution is also a Gaussian

$$P^*\left(\vec{\xi}\right) = (2\pi)^{-\mathcal{N}/2} \left(\det \mathbb{G}\right)^{-1/2} \exp\left[-\frac{1}{2} \sum_{\mu, v} \xi^\mu G_{\mu\nu} \xi^\nu \right] \ , \tag{D.2}$$

where

$$\mathbb{G} = \mathbb{C}^{-1}$$

with $\mathbb{C}$ being the correlation matrix:

$$\langle \xi^\mu \xi^\nu \rangle = C^{\mu\nu}.$$

The explicit form of $\mathbb{C}$ is found in the standard way, except that matrices are involved. Thus, it is formally

$$\mathbb{C} = \int \frac{d\omega}{2\pi} \left(\frac{1}{i\omega + \mathbb{F}} \right) \mathbb{N} \left(\frac{1}{i\omega + \mathbb{F}} \right)^\dagger$$

In the frame where $\mathbb{F}$ is diagonal, this integral is trivial. The result is, in terms of the explicit matrix elements:

$$C^{\mu\nu} = \sum_{I, J} \frac{u_I^\mu N^{IJ} u_J^\nu}{\lambda\left(I\right) + \lambda\left(J\right)} \ ,$$

where

$$N^{IJ} \equiv \sum_{\mu, v} v_\mu^I N^{\mu\nu} v_\nu^J$$

is just $\mathbb{N}$ in the new frame.

The probability currents are displayed in Equation (D.1):

$$K^\mu = -\sum_v \left\{ \frac{1}{2} N^{\mu\nu} \partial_\nu + F_\nu^\mu \xi^\nu \right\} P \ ,$$

so that the *stationary* currents are

$$K^{*\mu}\left(\vec{\xi}\right) = -\sum_v \left\{ \frac{1}{2} N^{\mu\nu} \partial_\nu + F_\nu^\mu \xi^\nu \right\} P^*\left(\vec{\xi}\right) \ .$$

To see that this is the (generalized) curl of a vector field, we exploit the Gaussian property of P^* and substitute

$$\xi^\gamma P^* = -\sum_v C^{\gamma\nu} \partial_\nu P^*$$

into the second term. Thus,

$$K^{*\mu}\left(\vec{\xi}\right) = \sum_v \left\{ \sum_\gamma F_\gamma^\mu C^{\gamma\nu} - \frac{1}{2} N^{\mu\nu} \right\} \partial_\nu P^*\left(\vec{\xi}\right).$$

Next, we want to show that the matrix in {...} is indeed antisymmetric. Recall that u is an eigenvector of F, so that

$$\sum_\gamma F_\gamma^\mu C^{\gamma\nu} = \sum_{I,J} \frac{\lambda(I)}{\lambda(I) + \lambda(J)} u_I^\mu N^{IJ} u_J^\nu .$$

For $N^{\mu\nu}$, we cast it in terms of N^{IJ}, i.e.,

$$N^{\mu\nu} = \sum_{I,J} u_I^\mu N^{IJ} u_J^\nu ,$$

so that the terms in {...} combine easily. The result is

$$K^{*\mu} = \sum_v A^{\mu\nu} \partial_\nu P^*$$

with

$$A^{\mu\nu} = \frac{1}{2} \sum_{I,J} \frac{\lambda(I) - \lambda(J)}{\lambda(I) + \lambda(J)} u_I^\mu N^{IJ} u_J^\nu ,$$

which is manifestly antisymmetric. Note that this $A^{\mu\nu}$ should not be confused with the A_i^j in Section 4.

[1] Schmittmann B and Zia R K P 1995 *Statistical Mechanics of Driven Diffusive Systems.* Vol. 17 of *Phase Transitions and Critical Phenomena*, eds. Domb C and Lebowitz J L (Academic, London).

[2] Mukamel D 2000, *Phase Transitions in Non-Equilibrium Systems*, in *Soft and Fragile Matter: Nonequilibrium Dynamics, Metastability and Flow*, eds. Cates M E and Evans M R (IOP Publishing, Bristol).

[3] The Isaac Newton Institute for Mathematical Sciences in Cambridge (UK) recently devoted one of its workshops to this problem. Webpostings of talks and papers can be found at http://www.newton.cam.ac.uk/programmes/PDS/index.html

[4] In the framework of the canonical ensemble, $\mathcal{H}$ is simply internal energy. For other ensembles, such as the grand-canonical ensemble, we will need to generalize our concept of reservoirs, and of the appropriate $\mathcal{H}$, but the key feature remains unchanged: Effectively, equilibrium systems are coupled to a *single* reservoir.

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